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ANALYSIS OF INDUSTRIAL WASTEWATER FOR ORGANIC POLLUTANTS IN CONSENT DECREE SURVEY

by

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16. ABSTRACT

In response to a need of the Effluent Guidelines Division of the U.S. EPA Office of Water Regulations and Standards, industrial wastewater survey sample extracts were analyzed for organic pollutants other than the Priority Pollutants. Chromatographic analyses were performed on capillary columns rather than the packed columns used in the original survey analysis to confirm compound identifications made by computer analysis of the packed column gas chromatography/mass spectrometry (GC/MS) data. A list of compound identifications for each industrial effluent extract to be analyzed was provided. These compounds were then obtained (if possible) either in-house or commercially from available sources for use as standards. Standards were analyzed and relative retention times, as well as relative molar response factors, were determined. In the first capillary GC/MS analysis of the industrial effluent extracts, a tentative identification of compounds of interest was made using all available resources (such as retention time relative to a standard, computerized or manual identification of the mass spectrum, or extracted ion current profiles). Where the compounds of interest were tentatively identified, quantities were calculated using the relative molar response factors. In a subsequent capillary GC/MS re-analysis of the industria effluent extract, tentative identifications were confirmed by spiking the extract with authentic compounds to observe coelution. Overall, 546 compounds were manually identified in the reanalysis of extracts. Of these, 433 were confirmed.

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FOREWORD

Nearly every phase of environmental protection depends on a capability to identify and measure specific pollutants in the environment. As part of this Laboratory's research on the occurrence, movement, transformation, impact, and control of environmental contaminants, the Analytical Chemistry Branch characterizes chemical constituents of water and soil.

In June 1976 the U.S. Environmental Protection Agency, as a result of court action by several environmental action groups, was directed by a Consent Decree from the U.S. District Court in the District of Columbia to assess the wastewater of 21 industrial categories for 65 chemical substances and prescribe the best available treatment for the effluent. The survey included analysis of samples by gas chromatography-mass spectrometry for 114 organic compounds considered to be priority pollutants. After the screening analysis for the 114 compounds, magnetic tapes containing raw data were computer analyzed to determine other compounds present. This report describes a program to confirm the computer identifications.

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ABSTRACT

In response to a need of the Effluent Guidelines Division of the U.S. EPA Office of Water Regulations and Standards, industrial wastewater survey sample extracts were analyzed for organic pollutants other than the Priority Pollutants. Chromatographic analyses were performed on capillary columns rather than the packed columns used in the original survey analysis to confirm compound identifications made by computer analysis of the packed column gas chromatography/mass spectrometry (GC/MS) data. A list of compound identifications for each industrial effluent extract to be analyzed was provided. These compounds were then obtained (if possible) either in-house or commercially from various repositories or from any other source for use as standards. Standards were analyzed and relative retention times, as well as relative molar response factors, were determined. In the first capillary GC/MS analysis of the industrial effluent extracts, a tentative identification of compounds of interest was made using all available resources (such as retention time relative to a standard, computerized or manual identification of the mass spectrum, or extracted ion current profiles). Where the compounds of interest were tentatively identified, quantities (in terms of ng/μL of extract) were calculated using the relative molar response factors. In a subsequent capillary GC/MS re-analysis of the industrial effluent extract, tentative identifications were confirmed by spiking the extract with authentic compounds to observe coelution. Overall, 546 compounds were manually identified in the reanalysis of extracts. Of these, 433 were confirmed. Due to lack of authentic standards, 100 compounds could not be confirmed. Of the total compounds tentatively identified, 13 were incorrectly identified by the computer match and manual identification.

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SECTION 1

INTRODUCTION

As a result of the June 1976 Consent Decree (1,2), EPA agreed to prescribe the best available treatment (BAT) for industrial wastes in 21 industrial categories. The chemical analysis program to support this work involved the analysis of over 4000 samples from 46 industrial categories and subcategories. Addressed specifically were 129 priority pollutants (114 organics, 13 metals, cyanide, asbestos). In March 1979, the Consent Decree was amended to include a new paragraph [4(c)] that required EPA to tentatively identify by spectrum matching and "analytically confirm" compounds not in the priority pollutant list and establish order-of-magnitude concentration levels.

After the screening analysis for the 114 organics, magnetic tapes containing the raw GC/MS data for each sample fraction and each corresponding sample fraction extract were sent to EPA's Athens Environmental Research Laboratory. There computerized analysis of the GC/MS data to determine compounds not on the 114-compound list was performed. After the computer analysis at the Athens laboratory, selected extracts were reanalyzed at the Research Triangle Institute to confirm the computer identifications. Although the computer program at Athens Environmental Research Laboratory provides an indication of a "level of confidence" for the compound identifications, a higher level of confidence than simple comparison of a mass spectrum with a mass spectral data base was desired. There are many factors in the overall analytical procedure that can contribute to the inability to make any compound identification at all or to making an incorrect identification, among them:

1) the analysis procedure (3) calls for the gas chromatographic analysis to be performed on packed columns. Aqueous industrial effluents are typically very complex samples and many components are unresolved in the elution from a packed column. In cases of multiple coelution, it is very difficult to deconvolute the data so that a clear, identifiable mass spectrum can be obtained for each coeluting component.

Thus, in subsequent computerized analysis of the data, the mass spectra either cannot be matched to the data base or are incorrectly matched.

2) the data base contains only mass spectra, with no information on elution order of compounds. Thus, in cases where members of a homologous series, for example, all have closely similar or identical mass spectra, the computer has no basis on which to select one homolog rather than another. A skilled human intterpreter, armed with information on relative retention times, can make a correct decision relatively easily, but the computerized data base is deprived of retention time information.

Also, quantitative data were obtained by using a simple ratio of system response for compound of interest to system response for a standard. When a higher level of certainty in compound identification and quantification was desired, the following modifications of the procedure were made: 1) extracts (stable under storage conditions, as opposed to volatiles) would be reanalyzed under capillary gas chromatography conditions. The additional resolution of components available under capillary chromatography conditions should yield mass spectra which could be identified more readily; 2) authentic standards of the compounds identified would be obtained and analyzed on the same capillary columns used for extract analysis. Relative retention time data would be available to be correlated with mass spectral data to enhance the certainty of compound identification; 3) relative molar response factors would be determined for the standard compounds so that accurate quantitation could be performed; 4) the optimum certainty in compound identification would be obtained by spiking the extracts with authentic standards of the compounds of interest to observe coelution of standard and tentatively identified compound with no change in the mass spectrum.

SECTION 2

PROCEDURE

Two gas chromatograph/mass spectrometer/computer systems were used in the original capillary analysis of the industrial effluent extracts. Compound identifications were confirmed on the same system which performed the original analysis. The LKB 2091 is a low resolution magnetic sector instrument; the Finnigan 3300 is a quadrupole with a mass range of 1000 daltons. On the LKB 2091, three capillary columns were used in the analysis of the industrial effluent extracts. The acid extracts were analyzed on a 50m Carbowax 20M, glass, wide-bore (0.5 mm), thick film (1μm) column. Base/neutral extracts were analyzed on a 50m SE-30, glass, wide-bore (0.5 mm), thick film (1 μm) column or a 25m CP-SIL-5 glass, wide-bore (0.5 mm) thick film (1μm) column. The CP-SIL-5 (a non-polar polydimethylsiloxane with high (80-100%) coating efficiency and temperature stability to 350°C with temperature programming) column was used in the analysis of extracts with late-eluting components such as polynuclear aromatic compounds for which retention times on the SE-30 column on this system were prohibitively long. Experimental work on the Finnigan 3300 was initiated approximately one year later than on the LKB system. In the interim, fused silica capillary columns became commercially available and this type of column was selected for use on the Finnigan system. For acid extracts, a 60m wide-bore (0.35 mm) thick film (1 μm) Carbowax 20M fused silica capillary column was used. For base/neutral extracts a 60m wide-bore (0.35 mm) thick film (1 μm) OV-101 fused silica capillary column was used. A third column for extracts containing late-eluting components proved to be unnecessary in this system since all of the polynuclear aromatic compounds which required confirmation would elute within 90 minutes on the column routinely used for base/neutral extracts. For operating conditions for the different columns and different systems, see Table 1.

Table 1. Instrument Operating Parameters

LKB 2091	
	Gas Chromatograph Parameters
Column	50M SE-30, wide-bore, thick film glass capillary
Initial Temperature	80°C
Minutes Isothermal	5
Programming Rate	5°C/min
Maximum Temperature	270°C
Column Flow	0.55 mL/min
Injector Temperature	240°C
Injection Mode	Split, ∿10:1
Column	25m CP-SIL-5, wide-bore, thick film glass capillary
Initial Temperature	120°C
Programming Rate	8°C/min
Maximum Temperature	300°C
Column Flow	0.84 mL/min
Injector Temperature	260°C
Injection Mode	Split, ∿10:1
Column	50m Carbowax 20M wide-bore, thick film glass capillary
Minutes Isothermal	6 at 80°C
Programming Rate	6°C/min
Maximum Temperature	220°C
Column Flow	0.58 mL/min
Injector Temperature	220°C
Injection Mode	Split, ∿10:1
	Mass Spectrometer Parameters
Transfer Line/Separator	280°C
Ionization Energy	70 eV
Trap Current	50 μA
Source Temperature	210°C
Accelerating Voltage	3.5 kV
Mass Range	6-492 daltons
Scan Speed	2 sec/cycle

(continued)

Table 1. (continued)

Finnigan 3300

	Gas Chromatograph Parameters
Column	60m OV-101 wide-bore, thick film fused silica capillary
Initial Temperature	30°C
Minutes Isothermal	6 minutes at 75°C
Programming Rate	4°C/min
Maximum Temperature	270°C
Column Flow	1.2 mL/min He
Injector Temperature	250°C
Injection Mode	Splitless for 60 seconds, then ~10:1 split
Column	60m Carbowax 20M wide-bore, thick film fused silica capillary
Initial Temperature	30°C
Minutes Isothermal	6 minutes at 75°C
Programming Rate	4°C/min
Maximum Temperature	220°C
Column Flow	1.2 mL/min He
Injector Temperature	250°C
Injection Mode	Splitless for 60 seconds, then ~10:1 split
	Mass Spectrometer Parameters
Transfer Line/Separator	270°C
Ionization Energy	70 eV
Emission Current	0.5 mA
Mass Range	40-500 daltons
Scan Speed	2 sec/cycle

Two internal standards were selected for calculation of relative retention times and relative molar response factors. Three primary criteria were employed in their selection: 1) they should be eluted in approximately the middle of the elution range; 2) they should be compounds not reasonably expected to occur in industrial effluents; and 3) they should exhibit simple mass spectra with unique masses which would not be confused with the masses of hydrocarbons and aromatic compounds found in industrial effluents. The two standards chosen were 4-fluoro-2-iodotoluene (PCR Research Chemicals, Inc., Gainesville, Florida; CAS Registry Number 13194-67-7) and 2-fluorobiphenyl (PCR Research Chemicals, Inc., Gainesville, Florida; CAS Registry Number 321-60-8). Mass spectra of these two compounds are shown in Figures 1 and 2. Both compounds have simple mass spectra, with masses unique in their retention windows. The presence of fluorine in the molecule enhances the volatility. The fluorinated molecule has a higher molecular weight but is eluted from the chromatographic column sooner than its hydrocarbon analog.

To monitor performance (and potential deterioration) of capillary columns as well as the tune of the mass spectrometer, a system performance solution was developed and analyzed at the start of each day. The composition of the system performance solution is shown in Table 2. Parameters measured and components used to measure them are:

1) column acidity/basicity: dimethylphenol and dimethylaniline.

2) resolution: octadecane and octadecene.

3) mass spectrometer tune: decafluorotriphenylphosphine.

4) GC/MS transfer line: methyl stearate and pyrene.

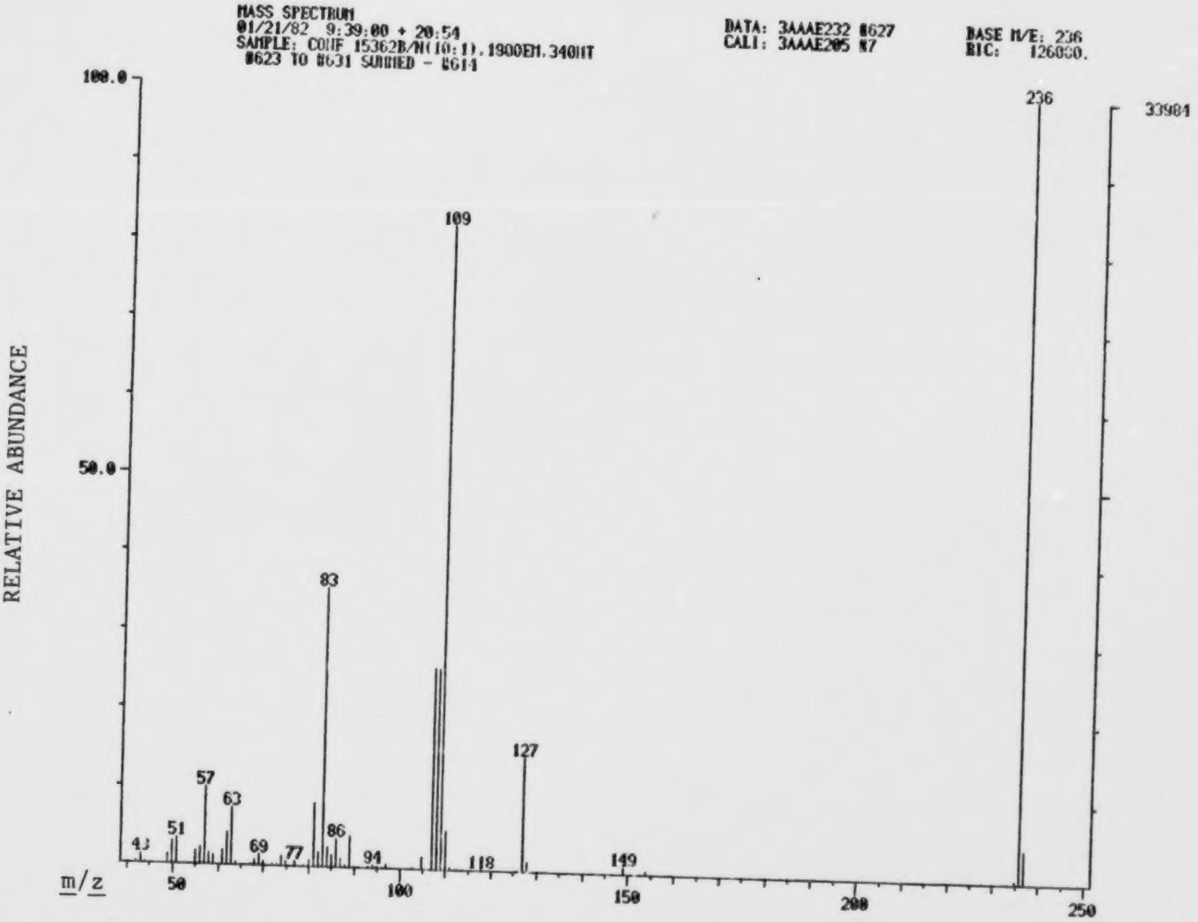

Figure 1. Mass spectrum of 4-fluoro-2-iodotoluene (CAS Registry Number 321-60-8).

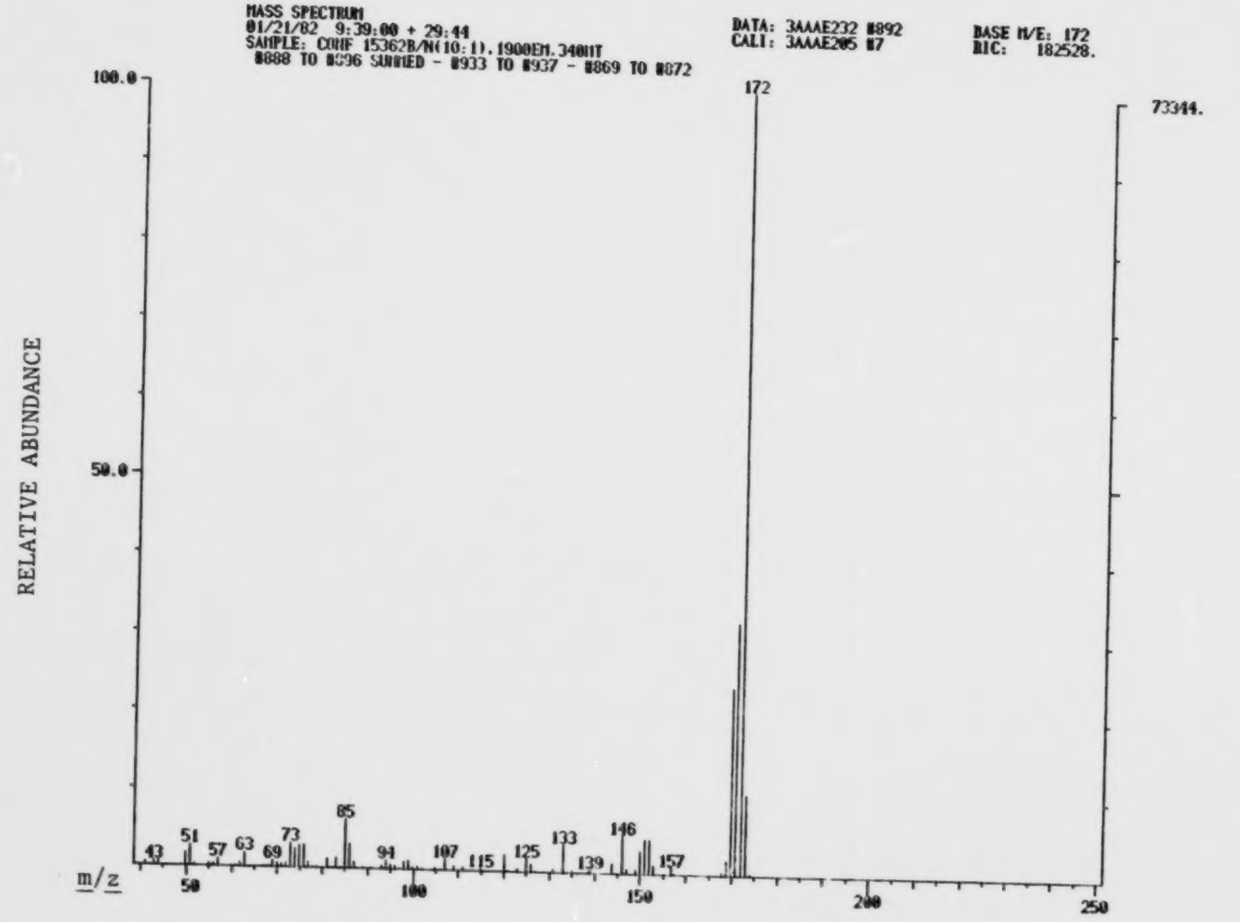

Figure 2. Mass spectrum of 2-fluorobiphenyl (CAS Registry Number 13194-67-7).

Table 2. Composition of System Performance Solutions

300 ng/μL in methylene chloride
2,6-dimethylaniline
2,6-dimethylphenol
2-ethylhexanoic acid
dicyclohexylamine
1-tetradecanol
acetophenone
100 ng/μL in methylene chloride
1-octadecene
octadecane
decafluorotriphenylphosphine
methyl stearate
eicosane
pyrene
heneicosane

5) column separation number: eicosane and heneicosane.

Further details may be found elsewhere (4).

No single specific compound was used as a special check on sensitivity. Overall and individual compound signal levels were monitored daily, however, and system sensitivity was assessed as a function of these signal levels. In addition to the above, ethylhexanoic acid and dicyclohexylamine were included to provide a more stringent test of column acidity/basicity by inspection; tetradecanol peak symmetry and signal level were monitored to check column activity. Columns were discarded and replaced with equivalents when acidity/basicity or resolution criteria could no longer be met. The tuning criteria for decafluorotriphenylphosphine are shown in Table 3. A representative decafluorotriphenylphosphine mass spectrum obtained during the analysis of the system performance solution is shown in Figure 3, with a listing of ion abundances in Table 4. The tuning criteria were met daily before any extract analyses were performed. A typical chromatogram of the system performance solution on the 60m OV-101 fused silica capillary column is shown in Figure 4; the peaks, in order of elution, are identified in Table 5. The comparable chromatogram on the 60m Carbowax 20M fused silica capillary column is shown in Figure 5 with peaks, in order of elution, identified in Table 6. Note that elution order differs on the two columns but the range of acceptability of performance parameters does not.

As a computerized list of compounds to be confirmed evolved, these compounds were targeted for acquisition as standards. Some of these compounds were available from in-house inventory, most were purchased commercially, some analyses of the industrial effluent extracts. A simple ratio of scan number for peak maxima was used to calculate relative retention time. In the original computerized analyses of data for the industrial effluent extracts, a "concentration" for a compound of interest was obtained from the ratio:

$$\text{"Concentration"} = \frac{\text{area of the base peak}}{\text{area } \underline{m}/\underline{z} \text{ 188 for } {}^{2}\text{H}_{10}\text{-anthracene}} \times \frac{\text{conc. of } {}^{2}\text{H}_{10}\text{-anthracene}}{\text{sample conc. factor}}$$

Table 3. Decafluorotriphenylphosphine Key Ions and Ion Abundance Criteria[a]

Mass	Ion Abundance Criteria
51	30-60% of mass 198
68	<2% of mass 69
70	<2% of mass 69
127	30-70% of mass 198
197	<1% of mass 198
198	base peak, 100% relative abundance
199	5-9% of mass 198
275	10-30% of mass 198
365	at least 1% of mass 198
441	present, but < mass 443
442	>40% of mass 198
443	17-23% of mass 442

[a] J. W. Eichelberger, L. E. Harris, and W. L. Budde, Anal. Chem., 47, 995 (1975).

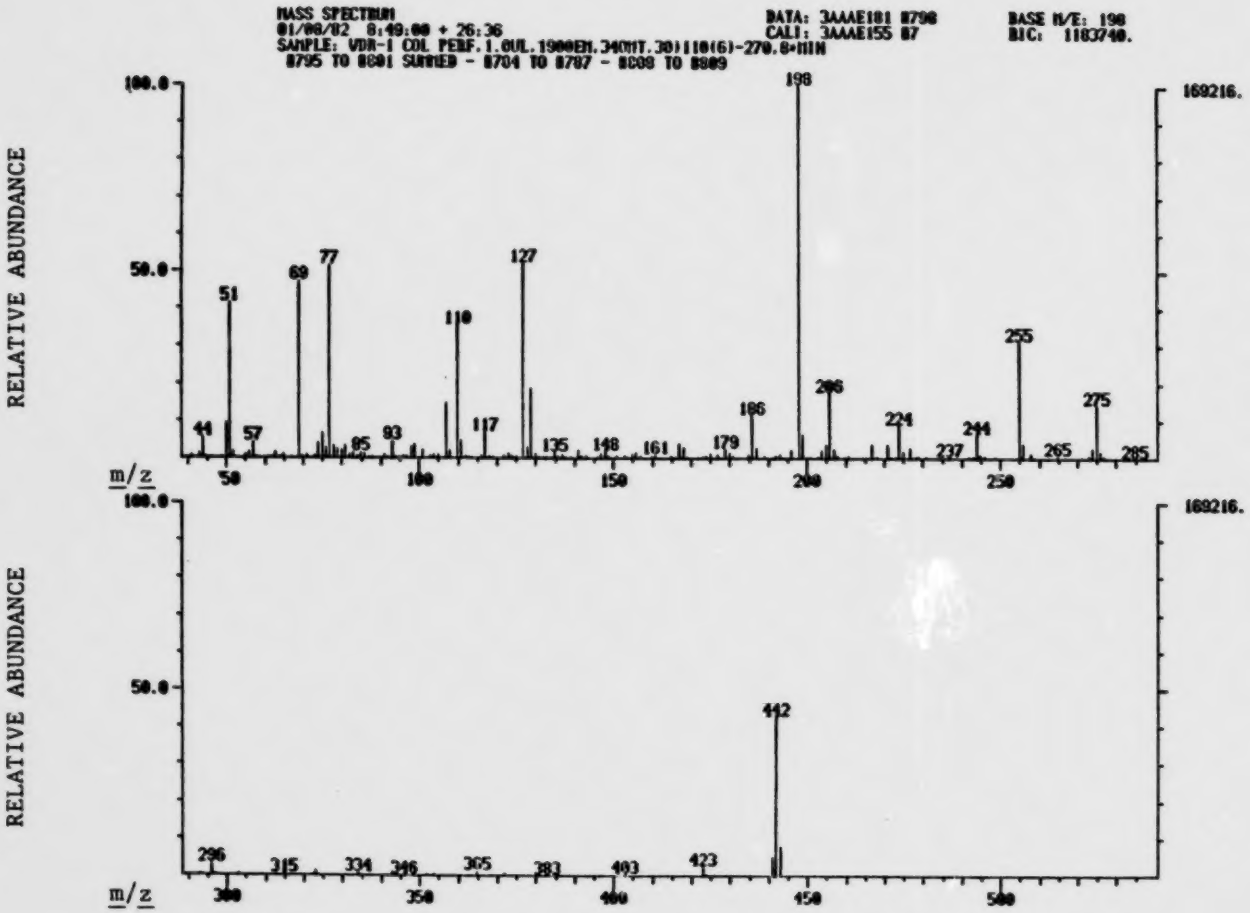

Figure 3. Representative mass spectrum of decafluorotriphenylphosphine.

Table 4. Representative Ion Abundances for Decafluorotriphenylphosphine

Mass	% RA	Mass	% RA
43	1.27	128	3.82
44	5.30	129	18.59
50	9.25	130	1.33
*51	41.53	135	1.54
52	1.87	137	0.89
55	0.96	141	2.10
56	1.55	142	0.62
57	4.36	147	1.26
63	1.51	148	1.82
65	0.84	149	0.75
69+	47.35	153	0.67
71	0.93	155	1.09
74	3.95	156	1.64
75	6.74	161	0.90
76	2.71	165	0.67
77	51.36	167	3.94
78	3.45	168	2.66
79	2.52	174	0.72
80	2.14	175	1.28
81	3.44	177	0.87
82	0.93	179	2.49
83	1.42	180	1.65
85	1.63	181	0.66
86	1.13	185	0.81
91	0.80	186	11.50
93	4.43	187	2.69
97	0.75	192	0.64
98	2.89	193	0.75
99	3.56	196	2.18
101	1.96	*198+	100.00
103	0.62	*199	6.26
104	0.92	204	2.14
105	1.02	205	3.63
107	14.88	206	17.53
108	2.11	207	2.42
110	35.48	217	3.55
111	4.67	221	3.74
117	6.99	224	8.60
122	0.75	225	1.86
123	1.32	227	2.78
125	0.70	244	6.29
*127	52.12	245	0.80

(continued)

Table 4. (continued)

Mass	% RA	Mass	% RA
246	0.61	277	0.68
255	31.32	296	2.94
256	3.93	323	1.08
258	1.31	*365	1.16
274	2.60	423	2.27
*275	14.28	*441	5.21
276	1.68	*442	42.89
		*443	7.43

[*] Key ions as specified in abundance criteria.

[+] Since m/z 68, 70, and 197 are <0.5% Relative Abundance, they are not included in this table.

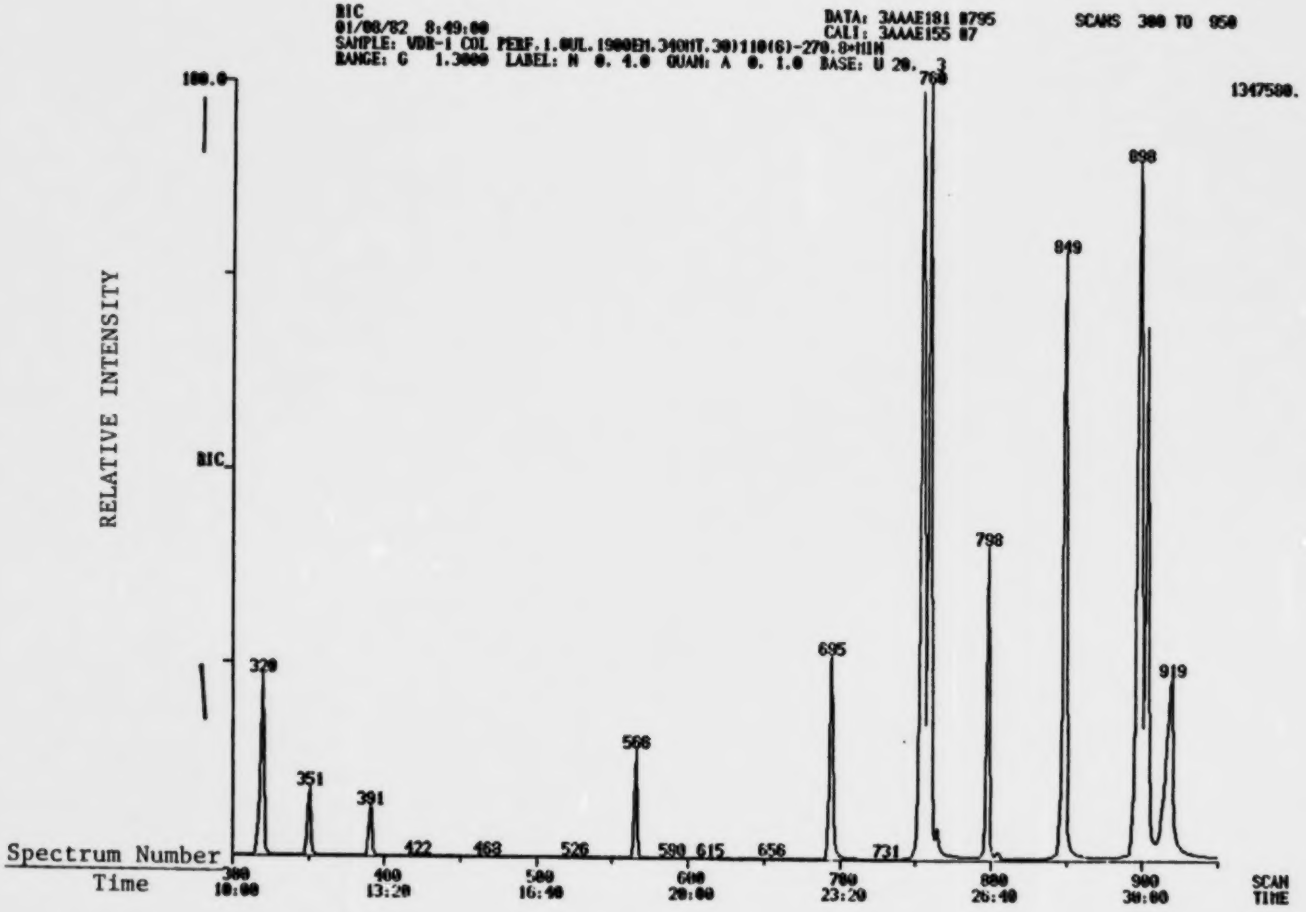

Figure 4. Typical chromatogram of system performance solution on the 60 m OV-101 fused silica capillary column. The programming rate was 8°C/min to minimize the time required for analysis.

Table 5. System Performance Solution Components in Order of Elution on OV-101 Column

Compound	Scan
acetophenone	320
2,6-dimethylphenol	351
2,6-dimethylaniline	391
dicyclohexylamine	566
1-tetradecanol	695
1-octadecene	755
octadecane	760
decafluorotriphenylphosphine	798
eicosane	849
heneicosane	898
methyl stearate	902
pyrene	919

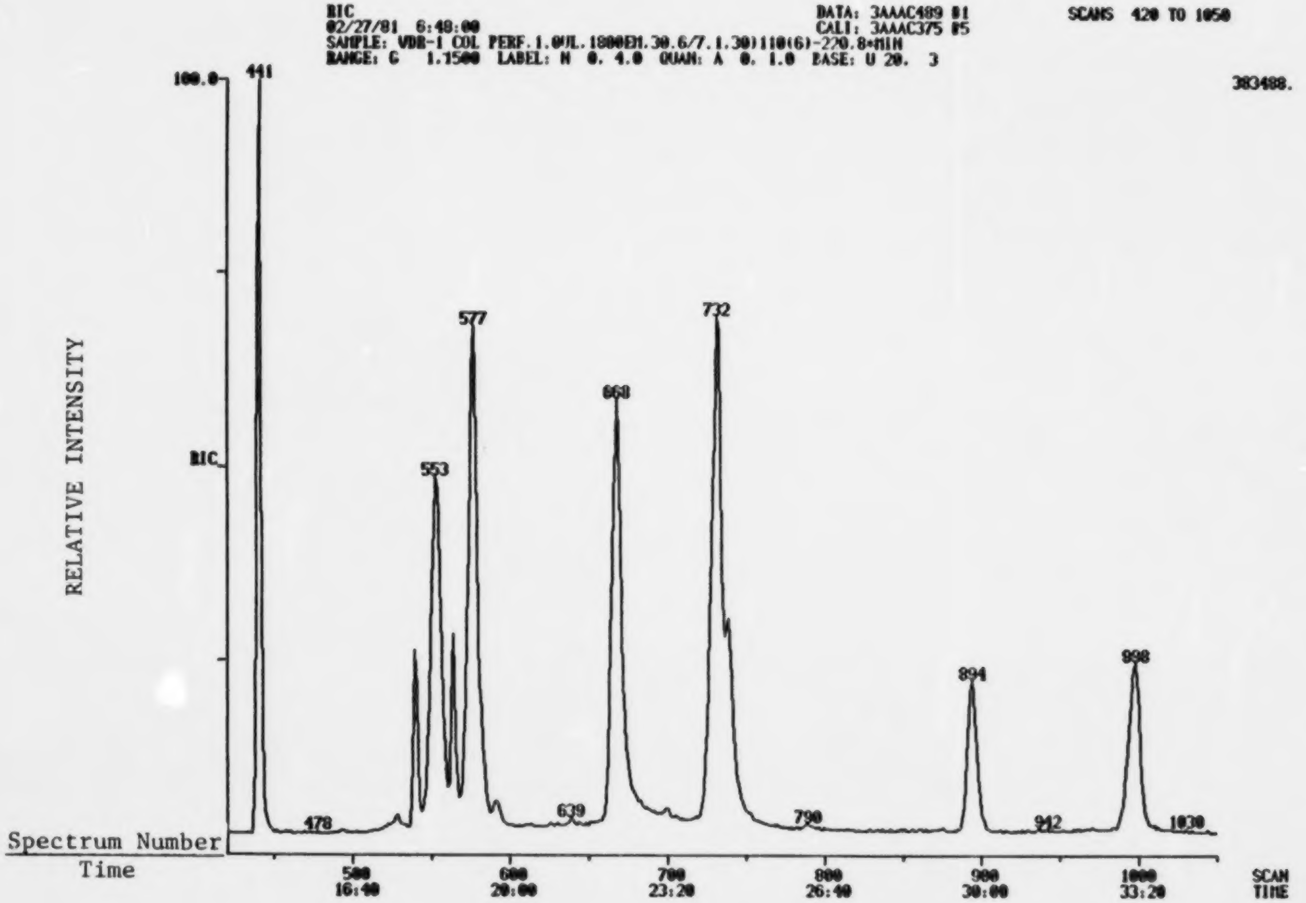

Figure 5. Typical chromatogram of system performance solution on the 60 m Carbowax 20M fused silica capillary column. The programming rate was 8°C/min to minimize the time required for analysis.

Table 6. System Performance Solution Components in Order of Elution on Carbowax 20M Column

Compound	Scan
acetophenone	441
2,6-dimethylaniline	540
2,6-dimethylphenol	564
octadecane	553
1-octadecene	577
eicosane	668
heneicosane	730
1-tetradecanol	739
decafluorotriphenylphosphine	894
methyl stearate[a]	998

[a] Pyrene does elute from the Carbowax 20M fused silica column but it has a very long retention time. The same performance solution was used for both columns, but since polar compounds were the primary interest on the Carbowax column, pyrene was disregarded and the peak asymmetry of methyl stearate was examined carefully.

In order to be able to perform more accurate quantitation, relative molar response factors were calculated for the standards. The reference compound chosen was 2-fluorobiphenyl (base peak m/z 172), with the option of using one of the ions from 4-fluoro-2-iodotoluene as a reference in the event of interference or other problems with fluorobiphenyl. With known quantities of compounds in methylene chloride solution, the relative molar response (RMR) factor was calculated as follows:

$$RMR = \frac{R_{cpd} \cdot moles_{std}}{R_{std} \cdot moles_{cpd}}$$

where

R = system response (peak height or peak area).

Relative retention times and relative molar response factors were obtained for well over six hundred compounds.

Analysis of industrial effluent extracts encompassed three major steps:

1) capillary GC/MS analysis of the extract for tentative identification of compounds to be confirmed, either manually or by computerized library search or by a combination of the two;
2) quantitation of compounds to be confirmed using relative molar response factors generated in the analysis of the standards;
3) confirmation of tentative identification by re-analysis of industrial effluent extracts spiked with standards.

To perform the initial capillary GC/MS analysis, the industrial effluent extract, appropriately diluted or concentrated as indicated by the computer-calculated "concentrations", was spiked at the level of ∿100 ng/μL with the two standards, 4-fluoro-2-iodotoluene and 2-fluorobiphenyl. The extract was then analyzed according to the appropriate conditions in Table 1, the mass spectrometer scanning continuously with the computer acquiring data. On the Finnigan 3300, most data interpretation was done on-line, using the computerized library search system. Spectra of major chromatographic peaks which could not be identified by the computer were output as hard copy for subsequent manual interpretation where possible. The LKB system is not equipped with computerized library search, so mass spectra of the major chromatographic components were output for subsequent manual interpretation. Several steps were required for compound identification:

1) Detection of compounds to be confirmed was assigned the highest priority. These could be major components of the chromatogram, minor components or, even under conditions of capillary chromatography, not well resolved from other components of the extract. Extracted ion current profiles were also used to aid in the location of compounds to be confirmed. On the basis of library search data, reverse search of the library , manual interpretation, extracted ion current profiles, and/or relative retention time information, a tentative identification of the compound was made or its apparent absence was reported.
2) In the computerized analysis of the data from the packed column chromatogram, compounds other than those to be confirmed had been tentatively identified. An effort was made, using the techniques described above, to re-identify these compounds. This level of compound identification, however, was assigned a lower priority than identification of compounds to be confirmed.
3) An effort was made to identify the major peaks of the chromatogram that did not fall into either of the above categories using either manual interpretation or computerized library search. This, obviously, could not be a major effort, since the overall objective of the program was not to characterize every extract completely.

Once compounds of interest had been tentatively identified, quantitative calculations were performed using the base peak of the mass spectrum of the compound of interest. A peak other than the base peak was used when necessary--for example, if the base peak happened to be saturated. Molar response factors relative to m/z 172 of the spectrum of 2-fluorobiphenyl were used together with the following equation to calculate nanogram of component per microliter of extract.

$$ng_u = \frac{R_u \cdot M_u \cdot ng_s}{R_s \cdot M_s \cdot RMR_{u/s}}$$

where

ng_u = number of nanograms of compound of interest

R_u = system response to the base peak of the mass spectrum of the compound of interest (peak height or peak area)

M_u = gram molecular weight of compound of interest

ng_s = number of nanograms of standard

R_s = system response to m/z 172 of 2-fluorobiphenyl (peak height or peak area)

M_s = gram molecular weight of standard

$RMR_{u/s}$ = relative molar response factor

Since the history of the samples (exact source, exact volume of water extracted, etc.) is confidential or not accessible, the simplest route to quantitation was to express the values as ng/μL extract, rather than ppm in the orginal water (the concentration factor from the original water sample is unknown; volumes were controlled at RTI). Some compounds were identified in industrial effluent extracts with no standards available to allow quantitation or confirmation of identification. In these cases, the identification was not confirmed but an approximate quantity could be estimated by using a relative molar response factor for a similar compound (preferably a positional isomer). In a few cases, standard compounds were available but could not be analyzed successfully in methylene chloride solution. Some compounds could be clearly identified in industrial effluent extracts but could not be analyzed successfully in standard solutions, possibly due to matrix effects in the extract or formation of these compounds from other components of the extract either in the injector or on-column. In these cases, the tentative identification of the compound could usually be confirmed by spiking into the industrial effluent extract but quantitation was approximate, relying upon the use of similar compounds.

At this point, with a tentative identification and a calculated quantity available for the compounds of interest, the industrial effluent extract could be spiked with an appropriate amount (usually 50-100% more than the calculated quantity) of standard material to allow confirmation of the identification by coelution. In many cases the confirmation of identification was straightforward - the correct compound was identified initially and, of course, coeluted clearly with the spiked material with no change in the mass spectrum. In some cases compounds were completely misidentified, both in the first computerized analysis and in the subsequent re-analysis. The situation of a misidentified compound became obvious when the standard material was spiked; a chromatographic peak appeared where none had been before. A situation far more common than complete misidentification, however, was that of misidentification of isomers, especially in the case of alkylated aromatic compounds. In these families of compounds, an entire series of isomers can have virtually identical mass spectra and, even under capillary chromatographic conditions, very closely similar elution times. Some coelute, even on a 50m capillary column (m- and p-xylene provide a specific example). Misidentification of isomers for these series constituted a chronic problem - in fact, correct original identification was rare (not too surprising, considering statistical probabilities). When standards were spiked and confirmation of identification was attempted, there were two possible outcomes:

1) the identification as a member of a certain family of compounds (for example, a C_4-alkylbenzene) was correct, but the particular isomer identified was simply not present; or
2) the particular peak tentatively identified was an incorrect isomer, but the correct isomer was present and could be identified after the standard was spiked. Where the correct isomer could be found, the peak position was reassigned and the quantity recalculated.

SECTION 3

RESULTS AND DISCUSSION

A total of 692 compounds was ultimately obtained and analyzed as a Standards Data Base (Appendix A). All of these compounds were analyzed on at least one column, some on two or three as tentative identifications seemed to warrant. A retention time relative to $^2H_{10}$-anthracene was obtained on every column where the compound was successfully analyzed to be consistent with the original EPA survey. Retention times relative to 2-fluorobiphenyl were obtained and used for Research Triangle Institute internal reference. In the original extracts d_{10}-anthracene was used as a reference. By the time the extracts were analyzed at the Research Triangle Institute, the d_{10}-anthracene could very seldom be found, nor could the oxidation product, the anthraquinone.

In the examination of the raw data from the original sample analysis, only about 5% of the data files were lacking d_{10}-anthracene. This discrepancy between the raw data and the reanalyzed sample extract is as yet unexplained. The Relative Molar Response factor, however, is based on *m/z* 172 of 2-fluorobiphenyl. Data for multiple analyses in Appendix A are indicative of crossover of compounds between fractions. This crossover is a measurement of the lack of effectiveness of the Priority Pollutant extraction scheme and/or the concentration level of the compound in the sample.

Appendix B includes lists of compounds (141) which were sought for use as standards but were not used because:

(1) the compound could not be chromatographed successfully after several attempts;

(2) the compound was not found in an extract and, being hazardous to handle, was therefore not chromatographed as a standard although it was in stock;

(3) some compounds were commercially available but their expense precluded their addition to the collection of standards, since they were not found in an extract.

(4) some compounds had no commercial or other known source. Of those in category (4), some were tentatively identified in extracts but the identification could not be confirmed.

Appendix C incorporates a table of industrial codes, including numerical codings and the number of extracts analyzed in each industrial code. Obviously, some industries are more extensively represented than others. The percent of the total number of extracts analyzed in this study for each industrial category is given in the right-hand column. Part of the problem with the lack of information for some of the industrial codes is that extracts were not supplied to the Environmental Protection Agency by the analytical laboratories responsible for procurement of the samples.

Appendix D is a compilation of compounds where identification was confirmed by coinjection of a standard, sorted according to CAS Registry Numbers and includes a number of occurrences of each compounds and the industrial codes where each occurrence has been verified. Compounds observed and verified the greatest number of times are shown in Table 7.

In order to understand the significance of the frequency of verified occurrences, a knowledge of the means for selection for verifiation is necessary. Compounds that were tentatively identified by the computer most often and in highest apparent concentration were chosen for verification. If a compound was found in more than one industrial category, an occurrence in one sample of each of these industrial categories was selected for verification. Thus, the occurrences verified indicate number of industrial categories in which the compound may be found. Most of the possible isomers (e.g., of the dimethylnaphthalenes) were observed when any members of the class were present. Concentrations of the compounds observed and verified are presented in Appendix E, sorted by industrial category. The uncertainties due to questionable documentation associated with the original sampling process, concentration, dilution, storage and extract degradation make conversion of RTI concentrations (in ng/μL extract) to ppm in the original water sample impractical. Appendix F gives an indication of the success rate of the confirmation process, with compounds ordered by CAS Registry Number within

Table 7. Compounds Verified Five or More Time

5 Occurrences

caffeine
2,3,4,6-tetrachlorophenol
fluorene
1,2,4,5-tetramethylbenzene
2,4,5-trichlorophenol
2-furaldehyde
nitrobenzene
p-dichlorobenzene
2-methyl-2,4-pentanediol
4-methyl-2-pentanone
heptanoic acid
2-(2-ethoxyethoxy)ethanol
methyl hexadecanoate
tributyl phosphate
dibenzothiophene
ethylbenzene
fluoranthene
acetovanillone
phenylpropionic acid
1-methyl-2-isopropylbenzene
9-methylphenanthrene
1-ethylnaphthalene
fenchyl alcohol
1-methylfluorene
4,7-dimethylindan

6 Occurrences

benzene
o-dichlorobenzene
p-*t*-butylphenol
m-toluic acid
n-propylbenzene
3,5-dimethylphenol
indole
s-butylbenzene
n-tricosane
1-methyl-3-ethylbenzene
1-methylphenanthrene
1,3-dimethyl-4-ethylbenzene

7 Occurrences

palmitic acid
1-hydroxy-2-phenylbenzene
acetophenone
butyric acid
nonanoic acid
vanillin
p-ethylphenol
pyrene
prehnitene
myristic acid
n-undecane
1-isopropyl-3,5-dimethylbenzene

8 Occurrences

biphenyl
benzothiazole
2,6-di-*t*-butyl-4-methylphenol
decanoic acid
borneol
1-methyl-3-isopropylbenzene
1-ethyl-2-*n*-propylbenzene

Table 7. (continued)

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9 Occurrences

phenanthrene
i-propylbenzene
p-cymene
styrene
diphenyl ether
1,3,5-trimethylbenzene
1,4-dimethylnaphthalene
2,3,5-trimethylnaphthalene

10 Occurrences

o-cresol
benzyl alcohol
phenylacetic acid
p-cresol
valeric acid
n-decane

11 Occurrences

benzoic acid
2-*n*-butoxyethanol
caprylic acid
caproic acid
lauric acid
1,6-dimethylnaphthalene
n-nonadecane

12 Occurrences

butyl phthalate
m-cresol
anthracene
2,3,6-trimethylnaphthalene
5-ethyl-*m*-xylene
2-ethylnaphthalene

13 Occurrences

n-eicosane
bis(2-ethylhexyl)phthalate
1,5-dimethylnaphthalene

14 Occurrences

o-xylene
1,2,4-trimethylbenzene
2-ethyl-1-hexanol
toluene
1,3-dimethylnaphthalene
n-tridecane
n-heptadecane

15 Occurrences

ethylbenzene
n-dodecane
1,2,3-trimethylbenzene
2,7-dimethylnaphthalene
1-methyl-3-ethylbenzene
p-ethyltoluene

Table 7. (continued)

16 Occurrences

α-terpineol
n-octadecane
1-methyl-2-ethylbenzene

17 Occurrences

p-xylene
m-xylene
tetrachloroethylene
n-tetradecane
n-pentadecane

18 Occurrences

1-methylnaphthalene

19 Occurrences

2-methylnaphthalene
phenol

20 Occurrences

n-hexadecane

22 Occurrences

1,8-dimethylnaphthalene

23 Occurrences

naphthalene

24 Occurrences

2-(2-butoxyethoxy)ethanol

confirmation percentage ranges. The first column of the table shows the number of times that a confirmation was requested. In the column headed % IND, the number of tentative identifications by RTI is given. % IND is the percentage of tentative identifications made in the number of times the compound was sought; the range is from 0 to 100. In the % CONF column, an entry indicates confirmation of the tentative identification. The % CONF column shows the success rate in the confirmation of tentative identifications, ranging again from 0-100%. The Table is sorted by increasing percentage of tentative identifications. Compounds which were sought the greatest number of times at RTI are tabulated below (Table 8) by chemical class, including number of tentative identifications and actual confirmations. Carboxylic acids are obviously well represented as a class in terms of number of occurrences but have a relatively low identification and, therefore, confirmation rate. In the majority of cases, when a compounds had been tentatively identified by RTI, the identification was confirmed. The aromatic acids also show a low rate of identification relative to the number of occurrences. Acid extracts were not derivatized prior to capillary analysis. Acid extracts had also been stored for periods as long as 2-3 years between the initial EPA contractor's analysis and the capillary analysis. There is always the possibility that the original acid simply was no longer present by the time the capillary analysis was performed. Alkanes and alkylbenzenes showed a high identification and confirmation rate, as did most of the alkylnaphthalenes. It is interesting to note that, in the case of 1,8-dimethylnaphthalene, the compound identification could be confirmed only once although 22 occurrences were noted. In the case of 1,7-dimethylnaphthalene and 1,3,6-trimethylnaphthalene, no confirmations at all could be made because standards were not available. The same situation (large number of occurrences, no standard available) occurs with 1- and 2-methylindan and 3-methylphenanthrene. The compound identification computer program apparently exhibits a bias in favor of tentative identification of the above isomers, since they are identified so frequently. This bias could be due both to the availability of reference spectra, and the fact that retention data for the isomers is indistinguishable on the packed columns used. It would seem that, if there is no commercial source for several of these isomers that are very frequently identified by the computer, the correctness of the identification should be questioned.

Table 8. Compounds with Ten or More EPA Tentative Identifications, with RTI Tentative Identification and Confirmation Rate

COMPOUND CLASS	EPA TENTATIVE IDENTIFICATIONS	RTI TENTATIVE IDENTIFICATION	CONFIRMATION
Carboxylic Acids (Aliphatic)			
butyric acid	10	7	7
valeric acid	12	10	10
hexanoic acid	17	11	11
caprylic acid	15	11	11
nonanoic acid	10	7	7
decanoic acid	13	8	8
lauric acid	16	12	11
myristic acid	18	7	7
palmitic acid	21	8	7
stearic acid	12	2	2
Carboxylic Acids (Aromatic)			
benzoic acid	26	11	11
m-toluic acid	11	7	6
phenylacetic acid	18	11	10
phenylpropionic acid	13	5	5
Alkanes			
n-decane	10	10	10
n-dodecane	20	17	15
n-tridecane	17	14	14
n-tetradecane	19	17	17
n-pentadecane	20	17	17
n-hexadecane	21	20	20
n-heptadecane	17	14	14
n-octadecane	20	16	16

Table 8. (continued)

COMPOUND CLASS	EPA TENTATIVE IDENTIFICATIONS	RTI TENTATIVE IDENTIFICATION	CONFIRMATION
n-nonadecane	14	11	11
n-eicosane	16	13	13
n-tricosane	11	6	6
Alkylbenzenes			
toluene	18	15	14
styrene	17	12	9
ethylbenzene	17	15	15
o-xylene	14	14	14
m-xylene	18	18	17
p-xylene	20	17	17
C_3-Alkylbenzenes			
1,2,4-trimethylbenzene	17	14	14
1,2,4-isopropylbenzene	16	10	9
1,3,5-trimethylbenzene	13	10	9
1,2,3-trimethylbenzene	18	16	15
1-methyl-2-ethylbenzene	18	17	16
1-methyl-3-ethylbenzene	16	15	15
p-ethyltoluene	20	16	15
C_4-Alkylbenzenes			
p-cymene	17	14	9
prehnitene	10	8	7
1-methyl-2-isopropylbenzene	14	10	5
1-methyl-3-isopropylbenzene	10	9	8
5-ethyl-m-xylene	14	12	12
1-methyl-2-n-propylbenzene	11	8	8
C_5-Alkylbenzenes			
1-isopropyl-3,5-dimethylbenzene	11	7	7

Table 8. (continued)

COMPOUND CLASS	EPA TENTATIVE IDENTIFICATIONS	RTI TENTATIVE IDENTIFICATION	CONFIRMATION
Alkylnaphthalenes			
naphthalene	25	23	23
1-methylnaphthalene	22	19	18
2-methylnaphthalene	21	19	19
C_2-Alkylnaphthalenes			
2-ethylnaphthalene	13	12	12
1,8-dimethylnaphthalene	22	14	1
1,4-dimethylnaphthalene	13	9	9
1,5-dimethylnaphthalene	16	13	13
1,7-dimethylnaphthalene	12	8	-[a]
1,3-dimethylnaphthalene	16	15	14
1,6-dimethylnaphthalene	12	11	11
2,7-dimethylnaphthalene	18	15	15
C_3-Alkylnaphthalenes			
2,3,6-trimethynaphthalene	17	12	12
2-isopropylnaphthalene	10	10	5
2,3,5-trimethylnaphthalene	14	11	9
1,3,6-trimethylnaphthalene	14	12	-[a]
Polynuclear Aromatic Compounds (and Miscellaneous Alkyl Aromatics)			
phenanthrene	16	9	9
anthracene	14	13	12
pyrene	13	7	7
fluoranthene	10	6	5
fluorene	11	6	5
biphenyl	13	8	8

Table 8. (continued)

COMPOUND CLASS	EPA TENTATIVE IDENTIFICATIONS	RTI TENTATIVE IDENTIFICATION	CONFIRMATION
2-methylanthracene	10	6	4
1-methylindan	11	8	-[a]
2-methylindan	10	8	-[a]
3-methylphenanthrene	11	6	-[a]
1-methylfluorene	11	6	5
Miscellaneous			
caffeine	11	7	7
α-terpineol	19	15	16
acetophenone	13	8	7
benzyl alcohol	13	11	10
2-ethyl-1-hexanol	21	16	14
vanillin	12	7	7
tetrachloroethylene	20	17	17
dibenzothiophene	11	5	5
2-n-butoxyethanol	16	11	11
2-(2-ethoxyethoxy)ethanol	10	5	5
2-(2-butoxyethoxy)ethanol	33	26	24
butyl phthalate	14	12	12
bis(2-ethylhexyl)phthalate	24	15	13
dioctyl phthalate	13	8	4

[a] Standard not available.

SECTION 4

RECOMMENDATIONS

Recommendations for further work in the characterization of components of aqueous industrial efflent extracts include:

- studies on the stability of the extracts themselves and on the stability of various compounds under the conditions of handling and storage to which these extracts are subjected. In many cases in the compound confirmation studies, a compound which should have been easily detected was simply not observed under capillary analysis conditions. One specific area of study would be the value of light shielding in preserving extract/compound integrity.
- incorporation of retention time data in the mass spectra data base to enhance the accuracy of computerized compound identification.
- better fractionation of extracts to reduce their complexity and the incidence of compound crossover: *i.e.*, hydrocarbons should not occur in the acidic fraction, phenolic compounds should not be found in the base/neutral fraction. More extensive fractionation (for example, applying the Master Analytical Scheme to the original water sample) would increase extract preparation time and the time required for analysis (more injections into the GC/MS system), but would significantly enhance the quality of data obtained.
- use of complementary analytical techniques, where feasible, to enhance the amount of information obtained from each sample could be very valuable. Examples are use of GC/Fourier transform infrared spectroscopy to produce information on functional groups, GC/high resolution mass spectrometry to deduce elemental composition, GC/chemical ionization mass spectrometry to enhance molecular weight information. Use of these techniques, however, presumes a desire to characterize hitherto uncharacterized components, rather than directly confirm a tentative identification.

REFERENCES

1. Settlement Agreement, NRDC *et al.* vs. EPA, U.S. District Court for the District of Columbia, June 7, 1976.
2. Joint Modification of Settlement Agreement, U.S. District Court for the District of Columbia, March 9, 1979.
3. Federal Register, December 3, 1979, p. 69464-69574.
4. "Master Analytical Scheme for the Analysis of Organic Compounds in Water. Volume III, Part I: Protocols" Draft final report, EPA contract No. 68-03-2704.

Appendix A

List of Standards

CASRN	Compound Name	GC	RRT*	RMR**
83329	ACENAPHTHENE	1	.7600	.3500
		2	.6100	.3500
208968	ACENAPHTHYLENE	1	.7200	.9000
		2	.6300	.7600
103844	ACETANILIDE	1	.6000	.0950
64197	ACETIC ACID	2	.2800	.0022
98862	ACETOPHENONE	1	.3800	.2600
		2	.3700	.3200
2478388	ACETOSYRINGONE	1	1.4600	.2200
		2	1.4200	.0740
1072839	2-ACETYLPYRROLE	1	.3800	.0460
		2	.5300	.2500
578950	ACRIDONE	3	1.5300	.0530
309002	ALDRIN	1	1.2400	.2400
		2	.8700	.3400
140670	P-ALLYLANISOLE	1	.4000	.2400
		2	.3200	.3100
2489863	1-ALLYLNAPHTHALENE	1	.7600	.4600
		2	.5900	.4100
99036	M-AMINOACETOPHENONE	1	.6700	.0560
		2	.9000	.0570
60093	4-AMINOAZOBENZENE(PHENYLAZOANILINE)	1	1.3000	.0170
118923	ORTHO-AMINOBENZOIC ACID(ANTHRANILIC ACID)	1	.7200	.0220
92671	4-AMINOBIPHENYL	1	.9420	.2000
		3	.9340	.0830
91598	2-AMINONAPHTHALENE	1	.8000	.2200
		2	1.0100	.0100
62533	ANILINE	1	.3000	.0500
		2	.4200	.1600
123115	P-ANISALDEHYDE	1	.5300	.1300

* Retention data relative to D10ANTHRACENE
** Relative to 2-fluorobiphenyl

GC Column Codes 1) 40 M SE-30 2) 50 M CARBOWAX 3) 25 M CP SIL-5

List of Standards

CASRN	Compound Name	GC	RRT*	RMR**
		2	.5800	.3600
105135	P-ANISYL ALCOHOL	1	.6000	.0350
		2	.6700	.1200
120127	ANTHRACENE	1	1.0000	.4200
		2	1.0000	.2800
84651	9,10-ANTHRAQUINONE	1	1.1700	.0700
		2	1.6500	.0400
		3	1.1900	.1400
1912249	ATRAZINE	1	.9290	.1800
103333	AZOBENZENE	1	.8700	1.1800
		2	.7200	.8900
100527	BENZALDEHYDE	1	.2800	.1000
		2	.3000	.1800
55210	BENZAMIDE	1	.6000	.1100
		2	.9600	.1100
93981	BENZANILIDE	1	1.1400	.0700
56553	1,2-BENZANTHRACENE	3	1.6000	2.7000
82053	BENZANTHRONE	3	1.6600	.1500
71432	BENZENE	1	.0610	.0710
		2	.0200	.0670
108985	BENZENETHIOL (THIOPHENOL)	1	.2900	.0810
		2	.3000	.0240
207089	11,12-BENZFLUORANTHENE	3	1.9900	.0890
230171	BENZO(C)CINNOLINE	1	1.1100	.0660
205992	BENZO(B)FLUORANTHENE	3	2.2400	.2800
243174	2,3-BENZOFLUORENE	1	1.5700	.2200
		3	1.4700	.6000
271896	BENZOFURAN	1	.3400	.2700
		2	.2900	.3100
65850	BENZOIC ACID	2	.8800	.0033
100470	BENZONITRILE (CYANOBENZENE)	1	.3000	.1900

* Retention data relative to D10ANTHRACENE
** Relative to 2-fluorobiphenyl

GC Column Codes 1) 40 M SE-30 2) 50 M CARBOWAX 3) 25 M CP SIL-5

List of Standards

CASRN	Compound Name	GC	RRT*	RMR**
		2	.3500	.4500
195197	3,4-BENZOPHENANTHRENE	3	1.7600	.8500
119619	BENZOPHENONE	1	.8600	.5200
		2	.7900	.6200
85029	5,6-BENZOQUINOLINE	1	1.0300	.2400
		2	1.2200	.2500
230273	7,8-BENZOQUINOLINE	1	1.0000	.5500
		2	1.0800	.4000
		3	1.0000	.5400
106514	P-BENZOQUINONE	1	.1700	.0700
95169	BENZOTHIAZOLE	1	.5400	.2800
		2	.5300	.4500
		3	.3800	.0780
95158	2,3-BENZOTHIOPENE (THIANAPHTHENE)	1	.5300	.8100
		2	.4500	.7100
50328	3,4-BENZPYRENE	3	2.2400	.0690
140114	BENZYL ACETATE	1	.3600	.3100
100561	PHENYLMERCURIC CHLORIDE	1	.8300	.0170
100516	BENZYL ALCOHOL	1	.4800	.1400
		2	.3600	.0530
100447	BENZYL CHLORIDE	1	.2900	.5100
538512	N-BENZYLIDENEPHENYLAMINE	1	.8900	.0430
		2	.7400	.3900
613592	2-BENZYLNAPHTHALENE	1	1.2700	.1100
92524	BIPHENYL	1	.6800	.8700
		2	.5400	.8900
259790	BIPHENYLENE	1	.7300	.3600
		2	.6000	.8300
111444	BIS(2-CHLOROETHYL)ETHER	1	.2500	.2100
		2	.2160	.5100
		3	.1500	.0098
128392	2,6-BIS(1,1-DIMETHYLETHYL)PHENOL	1	.7400	.1800

* Retention data relative to D10ANTHRACENE
** Relative to 2-fluorobiphenyl

GC Column Codes 1) 40 M SE-30 2) 50 M CARBOWAX 3) 25 M CP SIL-5

List of Standards

CASRN	Compound Name	GC	RRT*	RMR**
		2	.4070	.4400
106207	BIS(2-ETHYLHEXYL)AMINE	1	.8100	.0250
112492	1,2-BIS(METHOXYETHOXY)ETHANE	1	.5400	1.0100
		2	.4200	1.0400
6628188	1,2-BIS(METHYLMERCAPTO)ETHANE	1	.2500	.1200
507700	BORNEOL	1	.5000	.6100
		2	.3800	.4700
694804	1-BROMO-2-CHLOROBENZENE	1	.3900	.1000
108372	1-BROMO-3-CHLOROBENZENE	1	1.3900	.2100
19393921	1-BROMO-2,6-DICHLOROBENZENE	1	.6000	.3700
95567	ORTHO-BROMOPHENOL	2	.5100	.2200
106412	P-BROMOPHENOL	2	.8600	.0700
36563470	4-BROMOPHENYL PHENYL ETHER	1	.9100	.2200
		2	.7800	.2300
107926	BUTANOIC ACID (BUTYRIC ACID)	2	.3800	.0200
4170303	2-BUTENAL (CROTONALDEHYDE)	1	.0480	.0180
142961	1-BUTOXYBUTANE	1	.2100	1.1900
111762	2-BUTOXYETHANOL	1	.2100	.0400
		2	.2000	.4300
112345	2-(2-BUTOXYETHOXY)ETHANOL	1	.4900	.4500
		2	.4500	.6500
124174	2-(2-BUTOXYETHOXY)ETHYL ACETATE	1	.6500	.7000
		2	.4900	.9800
5131668	1-N-BUTOXYISOPROPANOL	1	.2500	.3700
		2	.1600	.4000
71363	N-BUTYL ALCOHOL	1	.0150	.0200
		2	.0250	.0690
25013165	BUTYLATED HYDROXY ANISOLE	2	.7900	.3200
103628	N-N-BUTYL-P-AMINOPHENOL	2	1.1900	.0037

* Retention data relative to D10ANTHRACENE
** Relative to 2-fluorobiphenyl

GC Column Codes 1) 40 M SE-30 2) 50 M CARBOWAX 3) 25 M CP SIL-5

List of Standards

CASRN	Compound Name	GC	RRT*	RMR**
104518	BUILYBENZENE	1	.3300	.7800
135988	SEC-BUTYLBENZENE	1	.3120	.1200
		2	.1100	.4200
98066	TERT-BUTYLBENZENE	1	.2930	.8800
		2	.1100	.5800
3622842	N-BUTYLBENZENESULPHONAMIDE	1	.9600	.1000
98737	P-TERT-BUTYLBENZOIC ACID	2	1.2100	.0065
85687	BUTYL BENZYL PHTHALATE	1	1.7700	.5600
		3	1.5600	.7900
2219821	6-TERT-BUTYL-M-CRESOL	2	.6700	.5100
513859	2,3-BUTYLENE GLYCOL	1	.1200	.2800
		2	.3300	.2300
142778	BUTYL OLEATE	1	1.5700	.0340
2876359	2-TERT-BUTYLNAPHTHALENE	1	.8000	2.7900
		2	.5700	2.4700
585342	M-TERT-BUTYLPHENOL	1	.5720	.2100
		2	.6300	.4600
88186	ORTHO-TERT-BUTYLPHENOL	1	.5400	.5900
		2	.6000	.8300
98544	P-TERT-BUTYLPHENOL	2	.6500	.5300
98511	4-T-BUTYLTOLUENE	1	.4400	.5600
		2	.1600	.3800
110656	BUTYNE-1,4-DIOL	2	.6800	.0025
58082	CAFFEINE	1	1.0100	.0800
79925	CAMPHENE	1	.3100	.4000
		2	.0480	.4000
502443	CAPROLACTONE	1	.4300	.1700
		2	.4900	.1800
86748	CARBAZOLE	1	1.0300	.2000
		3	1.0400	.2100

* Retention data relative to D10ANTHRACENE
** Relative to 2-fluorobiphenyl

GC Column Codes 1) 40 M SE-30 2) 50 M CARBOWAX 3) 25 M CP SIL-5

List of Standards

CASRN	Compound Name	GC	RRT*	RMR**
13466789	3-CARENE	1	.3500	.2900
		2	.0680	.3700
3734483	CHLORDENE (TENTATIVE FROM FIELD SAMPLES)	1	1.0200	.1000
		2	.7600	.0900
95512	2-CHLOROANILINE	1	.3900	.1300
108429	M-CHLOROANILINE	1	.5200	.0910
		2	.6100	.1700
619567	P-CHLOROBENZAMIDE	1	.7800	.0170
		2	1.4800	.0300
108907	CHLOROBENZENE	1	1.3900	.1400
535808	M-CHLOROBENZOIC ACID(3-CHLOROBENZOIC ACID)	1	.6500	.0220
		2	1.0600	.0240
118912	ORTHO-CHLOROBENZOIC ACID	1	.6800	.0240
		2	.9900	.0120
74113	P-CHLOROBENZOIC ACID	1	.6400	.0068
59507	4-CHLORO-M-CRESOL(4-CHLORO-3-METHYLPHENOL)	1	.5700	.1000
		2	.7200	.1600
29538770	TRANS-4-CHLOROCYCLOHEXANOL	1	.3200	.1600
		2	.4170	.3000
107142	CHLOROETHANENITRILE(CHLOROACETONITRILE)	1	.0160	.0080
67663	CHLOROFORM	1	.1000	.1400
86522	1-(CHLOROMETHYL)NAPHTHALENE	1	.8200	.5300
90131	1-CHLORONAPHTHALENE	1	.6800	.2800
		2	.5600	.2800
91587	2-CHLORONAPHTHALENE	1	.6900	.6400
		2	.5600	.5400
89634	4-CHLORO-2-NITROANILINE	1	.8300	.0500
		2	1.3200	.0390
121733	1-CHLORO-3-NITROBENZENE	1	.5500	.1700
		2	.5100	.2200
108430	M-CHLOROPHENOL	2	.7600	.1600

* Retention data relative to D10ANTHRACENE
** Relative to 2-fluorobiphenyl

GC Column Codes 1) 40 M SE-30 2) 50 M CARBOWAX 3) 25 M CP SIL-5

List of Standards

CASRN	Compound Name	GC	RRT*	RMR**
95578	ORTHO-CHLOROPHENOL	2	.4600	.2900
106489	P-CHLOROPHENOL	2	.7700	.2000
626608	3-CHLOROPYRIDINE	1	.1900	.0900
		2	.1800	.1300
897466	CHLOROTHALONIL	1	.9900	.1300
104825	ALPHA-CHLORO-P-XYLENE	1	.4600	.6200
		2	.3500	.6100
615601	4-CHLORO-ORTHO-XYLENE	1	.3800	.4300
218019	CHRYSENE	3	1.7100	.4000
470826	1,8-CINEOLE	1	.3600	.3600
		2	.0950	.3700
621829	CINNAMIC ACID	1	.7200	.0320
		2	1.0800	.0210
91645	COUMARIN	1	.7200	.0850
		2	.7800	.1600
95487	ORTHO-CRESOL	1	.3300	.1900
		2	.5200	.2800
108394	M-CRESOL	1	.3300	.1400
		2	.5500	.2200
106445	PARA-CRESOL (4-METHYLPHENOL)	1	.5000	.1500
		2	.5600	.3300
599644	4-CUMYLPHENOL	1	1.0400	.3900
294622	CYCLODODECANE	1	.6000	.5000
544252	CYCLOHEPTATRIENE	1	.1300	.1800
		2	.0440	.3500
98895	CYCLOHEXANECARBOXYLIC ACID	2	.5300	.0490
108930	CYCLOHEXANOL	1	.1900	.3600
		2	.2100	.2700
108941	CYCLOHEXANONE	1	.2200	.2500
		2	.1500	.8900

* Retention data relative to D10ANTHRACENE
** Relative to 2-fluorobiphenyl

GC Column Codes 1) 40 M SE-30 2) 50 M CARBOWAX 3) 25 M CP SIL-5

List of Standards

CASRN	Compound Name	GC	RRT*	RMR**
110838	CYCLOHEXENE	1	.0700	.3300
108918	CYCLOHEXYLAMINE (AMINOHEXAHYDROBENZENE)	1	.1300	.0073
527844	ORTHO-CYMENE	1	.3390	.2200
		2	.1700	.1900
706149	GAMMA-DECALACTONE	1	.7300	.0510
		2	.6300	.5900
112312	N-DECANAL	1	.4600	.2700
124185	N-DECANE	1	.3500	.8800
		2	.0350	.8600
334485	DECANOIC ACID	1	.5300	.1700
		2	.6400	.0800
112301	1-DECANOL(DECYL ALCOHOL)	1	.5800	.1900
		2	.4500	.1700
123422	DIACETONE ALCOHOL	1	.1500	.6300
		2	.1900	.4900
333415	DIAZINON	1	.9800	.2300
		2	.7800	.1600
262124	DIBENZO-P-DIOXIN	1	.8200	.6500
		2	.7100	.6200
132649	DIBENZOFURAN (DIPHENYLENE OXIDE)	1	.7700	.9200
132650	DIBENZOTHIOPHENE	1	.9700	.5100
		2	.9400	.4100
103491	DIBENZYLAMINE	1	.9300	.2900
		2	.7500	.0790
103504	DIBENZYL ETHER	1	.8600	.7500
35076927	1,4-DIBROMOCYCLOHEXANE	1	.5600	.4700
		2	.4300	1.1600
106934	1,2-DIBROMOETHANE	1	.1300	.1600
		2	.1300	.1800
111922	DI-N-BUTYLAMINE	1	.2900	.1200
		2	.0710	.0058

* Retention data relative to D10ANTHRACENE
** Relative to 2-fluorobiphenyl

GC Column Codes 1) 40 M SE-30 2) 50 M CARBOWAX 3) 25 M CP SIL-5

List of Standards

CASRN	Compound Name	GC	RRT*	RMR**
719222	2,6-DI-TERT-BUTYL-P-BENZOQUINONE	1	.7500	.2000
		2	.4900	.0120
		3	.6500	.1400
3905644	2,6-DI-TERT-BUTYLNAPHTHALENE	1	1.0800	.7300
128370	2,6-DI-TERTIARY-BUTYL-P-CRESOL (IONOL)	1	.7600	.8500
		2	.5000	1.3100
		3	.7000	.0830
96764	2,4-DI-TERT-BUTYLPHENOL	2	.6450	.1200
84742	DIBUTYL PHTHALATE	1	1.1300	.7600
		2	.9800	1.5500
534076	1,3-DICHLOROACETONE	1	.1100	.0770
608275	2,3-DICHLOROANILINE	1	.6200	.2700
		2	.7200	.3100
554007	2,4-DICHLOROANILINE	1	.6400	.1700
		2	.6600	.3500
95761	3,4-DICHLOROANILINE	1	.6600	.0330
541731	1,3-DICHLOROBENZENE	1	.3300	.4700
		2	.2200	.2700
95501	ORTHO-DICHLOROBENZENE	1	.3700	.4100
		2	.2800	.4300
106467	1,4-DICHLOROBENZENE	1	.3500	.3700
		2	.2600	.4100
51445	3,4-DICHLOROBENZOIC ACID	1	.7900	.0056
33284503	2,4-DICHLOROBIPHENYL	1	.8800	.4700
2050682	4,4'-DICHLOROBIPHENYL	1	.9900	.4000
19752557	1,3-DICHLORO-5-BROMOBENZENE	1	.5200	.3400
		2	.4000	.3100
764410	1,4-DICHLORO-2-BUTENE	1	.1900	.0700
1570656	4,6-DICHLORO-ORTHO-CRESOL	1	.5900	.2400
		2	.6600	.0370
822866	TRANS-1,2-DICHLOROCYCLOHEXANE	1	.3500	.3900

* Retention data relative to D10ANTHRACENE
** Relative to 2-fluorobiphenyl

GC Column Codes 1) 40 M SE-30 2) 50 M CARBOWAX 3) 25 M CP SIL-5

List of Standards

CASRN	Compound Name	GC	RRT*	RMR**
99309	2,6-DICHLORO-4-NITROANILINE	1	.9200	.0410
		2	1.3500	.0280
3209221	2,3-DICHLORONITROBENZENE	1	.6800	.1100
		2	.8500	.1100
120832	2,4-DICHLOROPHENOL	2	.6000	.1500
87650	2,6-DICHLOROPHENOL	2	.5400	.2000
94757	2,4-DICHLOROPHENOXYACETIC ACID(2,4-D)	1	1.0000	.0012
616239	2,3-DICHLORO-1-PROPANOL	1	.2000	.4000
		2	.4400	.0920
75990	2,2-DICHLOROPROPIONIC ACID (DALAPON)	1	.4200	.0025
95738	2,4-DICHLOROTOLUENE	1	.4700	.2900
		2	.3000	.2900
95750	3,4-DICHLOROTOLUENE	1	.4400	.3900
		2	.3600	.3100
111693	1,4-DICYANOBUTANE (ADIPONTRILE)	1	.4600	.0330
		2	.6500	.2200
101837	DICYCLOHEXYLAMINE	1	.7300	.6300
		2	.3800	.2100
60571	DIELDRIN	1	1.5400	.2800
111422	N,N-DIETHANOLAMINE	3	.2300	.0043
141935	M-DIETHYLBENZENE	1	.3490	.4700
		2	.1500	.3600
135013	1,2-DIETHYLBENZENE	1	.3490	.3500
		2	.1700	.0700
3352872	N,N-DIETHYLDODECANAMIDE	1	1.1200	.9700
		2	.7400	.9300
		3	1.1700	.9000
112367	DIETHYLENE GLYCOL DIETHYL ETHER	1	.2200	.1100
		2	.5700	.3200
104687	DIETHYLENE GLYCOL MONOPHENYL ETHER	1	.7700	.2800
		2	.8200	.4000

* Retention data relative to D10ANTHRACENE
** Relative to 2-fluorobiphenyl

GC Column Codes 1) 40 M SE-30 2) 50 M CARBOWAX 3) 25 M CP SIL-5

List of Standards

CASRN	Compound Name	GC	RRT*	RMR**
117817	DI-(2-ETHYLHEXYL)PHTHALATE	3	1.7500	1.6500
496162	2,3-DIHYDROBENZOFURAN	1	.4100	.2500
		2	.3400	.2700
496117	2,3-DIHYDROINDENE (INDAN)	1	.3800	.4100
		2	.2000	.3800
147477	1,2-DIHYDRO-2,2,4-TRIMETHYLQUINOLINE	1	.7400	1.0200
		2	.6000	1.2600
89849	2,4-DIHYDROXYACETOPHENONE	2	1.9100	.0120
105806	DIISOBUTYL AZELATE	1	1.7100	.3600
84695	DIISOBUTYL PHTHALATE	1	1.0400	.1200
		2	.8200	.1200
99627	1,3-DIISOPROPYLBENZENE	1	.5000	.7500
		2	.1900	.5500
100185	P-DIISOPROPYLBENZENE	1	.4700	.7000
2078548	2,6-DIISOPROPYLPHENOL	2	.5300	1.0400
91167	1,2-DIMETHOXYBENZENE (VERATROLE)	1	.4700	.3000
		2	.4100	.3300
150787	P-DIMETHOXYBENZENE	1	.4400	.4600
		2	.3500	.4100
2033898	3,4-DIMETHOXYPHENOL	2	1.0300	.0700
89747	2,4-DIMETHYLACETOPHENONE	1	.5300	.5200
		2	.4700	.3400
627930	DIMETHYL ADIPATE	1	.4900	.0650
121697	DIMETHYLANILINE	1	.4300	.3100
		2	.3200	.3000
781431	9,10-DIMETHYLANTHRACENE	1	1.4000	.3800
		3	1.3800	.5700
57976	9,10-DIMETHYL-1,2-BENZANTHRACENE	3	2.0900	.2900
603792	2,3-DIMETHYLBENZOIC ACID	2	1.0600	.0040
611018	2,4-DIMETHYLBENZOIC ACID	2	.9400	.0100

* Retention data relative to D10ANTHRACENE
** Relative to 2-fluorobiphenyl

GC Column Codes 1) 40 M SE-30 2) 50 M CARBOWAX 3) 25 M CP SIL-5

List of Standards

CASRN	Compound Name	GC	RRT*	RMR**
610720	2,5-DIMETHYLBENZOIC ACID	2	.8700	.0160
619045	3,4-DIMETHYLBENZOIC ACID	2	1.0100	.0066
499069	3,5-DIMETHYLBENZOIC ACID	1	.6500	.0520
		2	1.1200	.0036
612759	3,3'-DIMETHYLBIPHENYL	1	.8400	.1900
		2	.6600	.1600
613332	4,4'-DIMETHYLBIPHENYL	1	.8600	1.0600
		2	.6500	.8800
4706905	3,5-DIMETHYLCUMENE	1	.4500	.3100
624920	DIMETHYLDISULFIDE	1	.0650	.5600
933982	1,2-DIMETHYL-3-ETHYLBENZENE	1	.4080	1.0100
		2	.2200	.7000
2870044	1,3-DIMETHYL-2-ETHYLBENZENE	1	.3700	.7500
874419	1,3-DIMETHYL-4-ETHYLBENZENE	1	.3800	.5000
		2	.2000	.4200
68122	N,N-DIMETHYLFORMAMIDE	1	.0750	.0610
1119400	DIMETHYL GLUTARATE	1	.4400	.1600
		2	.4200	.1500
504201	2,6-DIMETHYL-2,5-HEPTADIEN-4-ONE (PHORONE)	1	.4200	.4900
		2	.2800	.4600
4912929	1,1-DIMETHYLINDAN	1	.3800	.0430
1685821	4,6-DIMETHYLINDAN	1	.5200	.6400
6682719	4,7-DIMETHYLINDAN	1	.6000	.5700
		2	.4000	.1400
91554	2,3-DIMETHYLINDOLE	1	.7700	.3400
		2	.8400	.3000
1196798	2,5-DIMETHYLINDOLE	1	.7500	.2000
		2	.6100	.1400
1459934	DIMETHYL ISOPHTHALATE	1	.7300	.0730
483783	1,6-DIMETHYL-4-ISOPROPYLNAPHTHALENE	1	.9100	.9800

* Retention data relative to D10ANTHRACENE
** Relative to 2-fluorobiphenyl

GC Column Codes 1) 40 M SE-30 2) 50 M CARBOWAX 3) 25 M CP SIL-5

List of Standards

CASRN	Compound Name	GC	RRT*	RMR**
		2	.6400	.8200
573988	1,2-DIMETHYLNAPHTHALENE	1	.7160	.7900
		2	.5500	.6700
575417	1,3-DIMETHYLNAPHTHALENE	1	.6860	.7000
		2	.5300	.4800
571584	1,4-DIMETHYLNAPHTHALENE	1	.7050	.5700
		2	.5700	.5200
571619	1,5-DIMETHYLNAPHTHALENE	1	.7050	.6800
		2	.5600	.6000
575439	1,6-DIMETHYLNAPHTHALENE	1	.6860	.5100
		2	.5500	.6700
569415	1,8-DIMETHYLNAPHTHALENE	1	.7330	.4400
		2	.6200	.3900
581408	2,3-DIMETHYLNAPHTHALENE	1	.7050	.3600
		2	.5800	.3400
581420	2,6-DIMETHYLNAPHTHALENE	1	.6740	.7800
		2	.5300	.5900
582161	2,7-DIMETHYLNAPHTHALENE	1	.6740	.5400
		2	.5400	.6900
1576698	2,7-DIMETHYLPHENANTHRENE	1	1.2700	.2600
		2	1.3200	.1800
1576676	3,6-DIMETHYLPHENANTHRENE	1	1.2500	.3900
		2	1.2900	.3100
526750	2,3-DIMETHYLPHENOL	2	.5700	.2500
		3	.2500	1.2800
95874	2,5-DIMETHYLPHENOL	1	.4480	.1400
		2	.5900	.3100
105679	2,4-DIMETHYLPHENOL	1	.4480	.1300
		2	.5900	.2600
95658	3,4-DIMETHYLPHENOL	1	.4600	.2000
576261	2,6-DIMETHYLPHENOL	1	.4030	.3000
		2	.4900	.2900
95658	3,4-DIMETHYLPHENOL	2	.6200	.1700

* Retention data relative to D10ANTHRACENE
** Relative to 2-fluorobiphenyl

GC Column Codes 1) 40 M SE-30 2) 50 M CARBOWAX 3) 25 M CP SIL-5

List of Standards

CASRN	Compound Name	GC	RRT*	RMR**
131113	DIMETHYL PHTHALATE	1	.7200	1.9900
		2	.6800	.2000
123320	2,5-DIMETHYLPYRAZINE	1	.2200	.2100
108509	2,6-DIMETHYLPYRAZINE	1	.2100	.2000
123320	2,5-DIMETHYLPYRAZINE	2	.1800	.1700
108509	2,6-DIMETHYLPYRAZINE	2	.1700	.1800
67516	3,5-DIMETHYLPYRAZOLE	1	.2780	.0640
108474	2,4-DIMETHYLPYRIDINE	1	.2400	.1400
		2	.1800	.1600
589935	2,5-DIMETHYLPYRIDINE	1	.1900	.1100
		2	.1800	.2400
108485	2,6-DIMETHYLPYRIDINE	1	.1900	.0740
		2	.1200	.0640
583584	3,4-DIMETHYLPYRIDINE	1	.3200	.2000
		2	.2800	.1600
591220	3,5-DIMETHYLPYRIDINE	1	.3000	.1300
		2	.2300	.2100
1198374	2,4-DIMETHYLQUINOLINE	1	.7200	.5200
		2	.6300	.5000
877430	2,6-DIMETHYLQUINOLINE	1	.6900	.6900
		2	.6100	.6300
67710	DIMETHYL SULFONE	1	.1900	.0510
		2	.5200	.1400
67685	DIMETHYL SULFOXIDE	1	.1100	.0280
		2	.3500	.0610
120616	DIMETHYLTEREPHTHALATE	1	.7100	.1600
13065071	2,7-DIMETHYL-1,2,3,4-TETRAHYDRONAPHTHALENE	1	.5800	.3800
126307	DIMETHYL TRIMETHYLENE GLYCOL	1	.2400	.1700
		2	.5600	.1400
2436966	2,2'-DINITROBIPHENYL	1	1.2600	.0810

* Retention data relative to D10ANTHRACENE
** Relative to 2-fluorobiphenyl

GC Column Codes 1) 40 M SE-30 2) 50 M CARBOWAX 3) 25 M CP SIL-5

List of Standards

CASRN	Compound Name	GC	RRT*	RMR**
		3	1.2500	.0600
99650	1,3-DINITROBENZENE	1	.7000	.0340
		2	.7700	.0410
1528741	4,4'-DINITROBIPHENYL	1	1.8800	.0100
121142	2,4-DINITROTOLUENE	1	.7600	.1800
606202	2,6-DINITROTOLUENE	1	.6900	.1800
		2	.6800	.1400
610399	3,4-DINITROTOLUENE	1	.7700	.0480
123795	DIOCTYL ADIPATE	2	1.1900	.7000
		3	1.6300	1.2200
117840	DIOCTYL PHTHALATE	1	1.6800	.0086
		3	1.8300	8.7100
123911	P-DIOXANE	1	.0290	.0120
882337	DIPHENYL DISULFIDE	1	1.0300	.2500
		2	.9400	.1400
612000	1,1-DIPHENYLETHANE	1	.7100	1.0700
587859	DIPHENYL MERCURY	1	1.1400	.2100
		3	1.1500	.0350
101815	DIPHENYLMETHANE	1	.7300	.6700
		2	.5500	.6100
139662	DIPHENYL SULFIDE	1	.7800	.4000
12002254	DIPROPYLENEGLYCOL METHYL ETHER	1	.2600	.2100
25265718	DIPROPYLENE GLYCOL	1	.3600	.0300
629970	N-DOCOSANE	1	1.5300	.7700
103195	DI-P-TOLYL DISULFIDE	1	1.2900	.1700
		2	1.2300	.0830
112403	N-DODECANE	1	.5400	1.1700
		2	.1100	.7900
112538	1-DODECANOL	1	.7400	.2000
		2	.5500	.1700

* Retention data relative to D10ANTHRACENE
** Relative to 2-fluorobiphenyl

GC Column Codes 1) 40 M SE-30 2) 50 M CARBOWAX 3) 25 M CP SIL-5

List of Standards

CASRN	Compound Name	GC	RRT*	RMR**
112414	1-DODECENE	1	.5300	.2500
		2	.1200	.1300
112958	N-EICOSANE	1	1.2200	1.3600
		2	.5500	2.0800
72208	ENDRIN	1	1.6200	.0051
		2	1.6100	.0028
96093	EPOXYETHYLBENZENE (STYRENE OXIDE)	1	.3800	.0790
		2	.3700	.1200
107211	1,2-ETHANEDIOL	1	.0410	.0006
		2	.3800	.0001
110805	2-ETHOXYETHANOL	1	.0590	.0200
		2	.0820	.1000
111159	2-ETHOXYETHANOL ACETATE	1	.2100	.1000
		2	.1600	.4200
112505	2(2-(2-ETHOXYETHOXY)ETHOXY)-ETHANOL	1	.5700	.6100
111900	2-(2-ETHOXYETHOXYETHANOL)	1	.3000	.3000
112505	2(2-(2-ETHOXYETHOXY)ETHOXY)-ETHANOL	2	.5600	.9200
111900	2-(2-ETHOXYETHOXYETHANOL)	2	.3500	.5900
52251715	2-ETHYLANTHRACENE	1	1.2400	.3600
		2	1.2800	.1300
		3	1.2400	.2100
53951501	AR-ETHYLBENZALDEHYDE	1	.4300	.1600
100414	ETHYLBENZENE	1	.2100	.3600
		2	.0620	.4000
103366	ETHYL CINNAMATE	1	.7100	.5200
1678917	ETHYLCYCLOHEXANE	1	.1300	.2500
110383	ETHYL DECANOATE	1	.6500	.8500
2008415	S-ETHYLDIISOBUTYLTHIOCARBAMATE (SUTAN)	1	.7100	.3000
		2	.4400	.3700
759944	S-ETHYL DIPROPYL THIOCARBAMATE (EPTC)	1	.6300	.4600

* Retention data relative to D10ANTHRACENE
** Relative to 2-fluorobiphenyl

GC Column Codes 1) 40 M SE-30 2) 50 M CARBOWAX 3) 25 M CP SIL-5

List of Standards

CASRN	Compound Name	GC	RRT*	RMR**
		2	.4100	.6300
104767	2-ETHYL-1-HEXANOL	1	.3500	.7300
		2	.2800	.5400
106332	ETHYL LAURATE	1	.8100	1.1800
		2	.4100	.7800
529215	3-ETHYL-4-METHYLPYRIDINE	1	.4100	.1700
		2	.3300	.1600
124061	ETHYL MYRISTATE	1	.9900	.6900
1127760	1-ETHYLNAPHTHALENE	1	.6650	.7300
		2	.5200	.7000
939275	2-ETHYLNAPHTHALENE	1	.6650	.1300
		2	.4570	.5400
106321	ETHYL N-OCTANOATE	1	.4700	.6600
628977	ETHYL PALMITATE	1	1.2200	1.0700
620177	META-ETHYLPHENOL	2	.6300	.0300
90006	ORTHO-ETHYLPHENOL	1	.4360	.2800
		2	.5500	.3200
123079	P-ETHYLPHENOL	1	.4710	.1500
		2	.6000	.5200
84662	ETHYL PHTHALATE	1	.8200	.5500
		2	.7200	.5600
104905	5-ETHYL-2-PICOLINE	1	.2900	.3000
		2	.2400	.2900
13925003	ETHYLPYRAZINE	1	.2300	.0690
		2	.1800	.1000
100710	2-ETHYLPYRIDINE	1	.2400	.2500
		2	.1400	.3800
536754	4-ETHYLPYRIDINE	1	.3000	.0680
		2	.2100	.1500
2896608	4-ETHYLRESORCINOL	1	.6800	.0420
620144	M-ETHYLTOLUENE	1	.2570	.7600

* Retention data relative to D10ANTHRACENE
** Relative to 2-fluorobiphenyl

GC Column Codes 1) 40 M SE-30 2) 50 M CARBOWAX 3) 25 M CP SIL-5

List of Standards

CASRN	Compound Name	GC	RRT*	RMR**
		2	.1000	.5000
80397	N-ETHYL-P-TOLUENESULFONAMIDE	1	.8800	.2600
		3	.8800	.2000
3982670	1-ETHYL-2,4,6-TRIMETHYLBENZENE	1	.4900	.7800
934805	4-ETHYL-ORTHO-XYLENE	1	.3860	.0700
		2	.2000	.5700
934747	5-ETHYL-M-XYLENE	1	.3570	.8400
		2	.0170	.6400
97530	EUGENOL	1	.6300	.1300
		2	.5900	.2300
1195795	FENCHONE	1	.4100	.3200
		2	.2100	.5700
1632731	FENCHYL ALCOHOL	1	.4300	.3200
		2	.3300	.3200
86737	FLUORENE (2,3-BENZINDENE)	1	.8400	.8600
206440	FLUORANTHENE	1	1.3600	.3400
86737	FLUORENE (2,3-BENZINDENE)	2	.7000	.6100
486259	FLUORENONE	1	.9500	.5300
		2	1.0300	.3200
367124	ORTHO-FLUOROPHENOL	2	.3710	.2100
98011	2-FURALDEHYDE	1	.1600	.0021
		2	.2700	.1200
620020	5-METHYL-2-FURANCARBOXALDEHYDE	1	.2400	.0610
98000	FURFURYL ALCOHOL	1	.1600	.0290
		2	.3700	.0700
629947	N-HENEICOSANE	1	1.4000	.1600
		2	.5700	.4100
1024573	HEPTACHLOR EPOXIDE	1	1.3000	.1400
593497	N-HEPTACOSANE	3	1.9900	.6300
629787	N-HEPTADECANE	1	.9300	.7600

* Retention data relative to D10ANTHRACENE
** Relative to 2-fluorobiphenyl

GC Column Codes 1) 40 M SE-30 2) 50 M CARBOWAX 3) 25 M CP SIL-5

List of Standards

CASRN	Compound Name	GC	RRT*	RMR**
		2	.4000	1.4100
111717	HEPTANAL	1	.1400	.0084
111148	HEPTANOIC ACID	2	.5200	.0800
110430	HEPTAN-2-ONE	1	.2200	.2500
118741	HEXACHLOROBENZENE	1	.9400	.2700
		2	.6700	.2200
87683	1,3-HEXACHLOROBUTADIENE	1	.5500	.7100
		2	.2800	.3400
58899	GAMMA-1,2,3,4,5,6-HEXACHLOROCYCLOHEXANE	1	.9590	.1600
67721	HEXACHLOROETHANE	1	.4200	.3700
		2	.2300	.2700
630013	N-HEXACOSANE	2	.9100	.5100
		3	1.8100	1.0300
544763	N-HEXADECANE	1	.8500	.8400
		2	.3500	1.3300
36653824	1-HEXADECANOL	1	1.0700	.0830
		2	.7400	.1700
629732	1-HEXADECENE	1	.8400	.9100
		2	.3700	.6200
142621	HEXANOIC ACID(CAPROIC ACID)	1	.2900	.0840
		2	.4500	.0800
112594	2-(2-HEXOXYETHOXY)ETHANOL	1	.6600	.5900
		2	.5500	.8200
112254	2-HEXYLOXYETHANOL	1	.4200	.3000
		2	.3500	.6100
118934	ORTHO-HYDOXYACETOPHENONE	2	.4500	.3700
123080	P-HYDROXYBENZALDEHYDE	2	1.3200	.0200
1137424	P-HYDROXYBENZOPHENONE	1	1.2200	.0087
934349	2-HYDROXYBENZOTHIAZOLE	1	.8800	.0300
1953544	5-HYDROXYINDOLE	1	.8500	.0140

* Retention data relative to D10ANTHRACENE
** Relative to 2-fluorobiphenyl

GC Column Codes 1) 40 M SE-30 2) 50 M CARBOWAX 3) 25 M CP SIL-5

List of Standards

CASRN	Compound Name	GC	RRT*	RMR**
499752	2-HYDROXY-4-ISOPROPYL-1-METHYLBENZENE	2	.6500	.2400
498022	4-HYDROXY-3-METHOXYACETOPHENONE	1	.7300	.1900
		2	.8200	.1800
621590	3-HYDROXY-4-METHOXYBENZALDEHYDE	1	.7400	.0600
		2	.9800	.0600
		3	.5100	.0100
306081	4-HYDROXY-3-METHOXYPHENYLACETIC ACID	1	.9300	.0064
148243	8-HYDROXYQUINOLINE	1	.6600	.1300
		2	.7600	.0040
6753986	HUMULENE	1	.6100	.5300
		3	.6400	.9000
83330	INDAN-1-ONE	1	.5900	.2100
		2	.5500	.2400
95136	INDENE	1	.3400	.5100
120729	INDOLE	2	.7500	.3300
		1	.6100	.1300
879378	3-INDOLEACETAMIDE	3	1.2600	.0390
540385	P-IODOPHENOL	1	.6400	.1400
		2	1.0700	.1100
124765	ISOBORNEOL	1	.5000	.4900
		2	.3800	.4900
79312	ISOBUTYRIC ACID	2	.3400	.0400
491305	ISOCARBOSTYRIL	1	.9800	.0190
		3	.9000	.0290
97541	ISOEUGENOL	1	.7000	.1600
		2	.6900	.1900
78591	ISOPHORONE	1	.4400	.7900
		2	.3400	.6800
98828	ISOPROPYLBENZENE (CUMENE)	1	.2200	.1100
		2	.0850	.3300
696297	ISOPROPYLCYCLOHEXANE	1	.2000	.1900

* Retention data relative to D10ANTHRACENE
** Relative to 2-fluorobiphenyl

GC Column Codes 1) 40 M SE-30 2) 50 M CARBOWAX 3) 25 M CP SIL-5

List of Standards

CASRN	Compound Name	GC	RRT*	RMR**
2027170	2-ISOPROPYLNAPHTHALENE	1	.7500	.6700
		2	.5500	.4100
618451	META-ISOPROPYLPHENOL	1	.5300	.0870
		2	.6200	.3200
88697	ORTHO-ISOPROPYLPHENOL	1	.4700	.3500
		2	.5700	.6700
99898	P-ISOPROPYLPHENOL	2	.6700	.2000
119653	ISOQUINOLINE	1	.5800	.0830
		2	.5300	.3500
143077	LAURIC ACID (N-DODECANOIC ACID)	1	.6500	.1400
		2	.8000	.0350
475207	LONGIFOLENE	1	.7000	.2500
5989275	(+)-P-MENTHA-1,8-DIENE (D-LIMONENE)	1	.3300	.5400
		2	.1000	.3500
1490046	MENTHOL	1	.3900	.2500
68111	2-MERCAPTOETHANOIC ACID(THIOGLYCOLIC ACID)	1	.3000	.0035
487683	MESITALDEHYDE	1	.6100	.5200
		2	.4800	.5000
79414	METHACRYLIC ACID	2	.4100	.0100
104949	4-METHOXYANILINE(P-ANISIDINE)	1	.5300	.1000
		3	.3500	.0930
109864	2-METHOXYETHANOL	1	.0310	.0600
		2	.0620	.1700
111773	2-(2-METHOXYETHOXY)ETHANOL	1	.2300	.1100
		2	.3300	.3800
110496	2-METHOXYETHYL ACETATE	1	.1400	.1900
121346	3-METHOXY-4-HYDROXYBENZOIC ACID	1	.8600	.0160
110430	HEPTAN-2-ONE	2	.0780	.3600
107982	1-METHOXYISOPROPANOL	1	.0450	.3300
		2	.0430	.4300

* Retention data relative to D10ANTHRACENE
** Relative to 2-fluorobiphenyl

GC Column Codes 1) 40 M SE-30 2) 50 M CARBOWAX 3) 25 M CP SIL-5

List of Standards

CASRN	Compound Name	GC	RRT*	RMR**
90051	ORTHO-METHOXYPHENOL	1	.3400	.1600
		2	.4700	.2600
577162	ORTHO-METHYLACETOPHENONE	1	.4600	.1400
150765	P-METHOXYPHENOL	1	.5300	.0960
577162	ORTHO-METHYLACETOPHENONE	2	.4100	.2200
150765	P-METHOXYPHENOL	2	.7000	.2300
100618	N-METHYLANILINE	1	.3900	.0690
		2	.4300	.2200
610480	1-METHYLANTHRACENE	1	1.1300	.7700
		2	1.1800	.1700
613127	2-METHYLANTHRACENE	1	1.1400	1.4200
		2	1.1500	1.3400
779022	9-METHYLANTHRACENE	1	1.1900	.7500
2319962	5-METHYLBENZO(A)ANTHRACENE	3	1.8600	.0710
2541697	7-METHYLBENZO(A)ANTHRACENE	3	1.8400	.2200
2381160	9-METHYLBENZO(A)ANTHRACENE	3	1.7100	1.1700
2581319	12-METHYLBENZO(A)ANTHRACENE	3	1.8600	.3800
93583	METHYL BENZOATE	1	.4100	.3700
		2	.3700	.3200
99945	P-METHYLBENZOIC ACID	2	.0840	.0110
120752	2-METHYLBENZOTHIAZOLE	1	.6100	.3700
		2	.5400	.2900
89952	ORTHO-METHYLBENZYL ALCOHOL	1	.4500	.1800
		2	.5400	.3100
643583	2-METHYLBIPHENYL	1	.6800	.7100
		2	.5000	.7000
123513	3-METHYL-1-BUTANOL	1	.0610	.2200
115195	2-METHYL-3-BUTYN-2-OL	1	.0320	.0340
		2	.0810	.2000

* Retention data relative to D10ANTHRACENE
** Relative to 2-fluorobiphenyl

GC Column Codes 1) 40 M SE-30 2) 50 M CARBOWAX 3) 25 M CP SIL-5

List of Standards

CASRN	Compound Name	GC	RRT*	RMR**
110429	METHYL CAPRATE	1	.6000	.5100
		2	.2800	.5500
110496	2-METHOXYETHYL ACETATE	2	.1300	.3700
1484124	9-METHYLCARBAZOLE	1	1.0400	.2300
95498	1-METHYL-2-CHLOROBENZENE (ORTHO-CHLOROTOLUENE)	1	.2900	.5800
		2	.1600	.5200
108418	1-METHYL-3-CHLOROBENZENE (M-CHLOROTOLUENE)	1	.2700	.4800
		2	.1600	.4200
3697243	5-METHYLCHRYSENE	3	1.8600	.3000
589924	4-METHYLCYCLOHEXANONE	1	.2300	.3700
2758181	3-METHYLCYCLOPENT-2-ENE-1-ONE	1	.3000	.0350
		2	.2900	.0900
6975980	2-METHYLDECANE	1	.4200	1.0500
		2	.0410	1.0700
2847725	4-METHYLDECANE	1	.4000	.3700
		2	.0400	.4000
874351	5-METHYL-(2,3-DIHYDROINDENE)(5-METHYLINDAN)	1	.4100	.1400
2467029	2,2-METHYLENEDIPHENOL	1	1.1800	.0310
203645	4,5-METHYLENEPHENANTHRENE	1	1.1300	.7100
		2	1.2100	.4200
80057	4,4'-(1-METHYLETHYLIDENE)BISPHENOL	1	1.4900	.0270
611143	1-METHYL-2-ETHYLBENZENE (O-ETHYLTOLUENE)	1	.2750	.5200
		2	.1200	.3500
622968	1-METHYL-4-ETHYLBENZENE (P-ETHYLTOLUENE)	1	.2590	.7800
		2	.0990	.3600
1730376	1-METHYLFLUORENE	1	.9300	.6200
		2	.7900	.6200
1430973	2-METHYLFLUORENE	1	.9300	1.0300
		2	.7700	.6500
1556996	4-METHYLFLUORENE	1	.9400	.3400

* Retention data relative to D10ANTHRACENE
** Relative to 2-fluorobiphenyl

GC Column Codes 1) 40 M SE-30 2) 50 M CARBOWAX 3) 25 M CP SIL-5

List of Standards

CASRN	Compound Name	GC	RRT*	RMR**
		2	.8100	.2900
821556	METHYL HEPTYL KETONE	1	.3100	.4600
112390	METHYL HEXADECANOATE(METHYL PALMITATE)	1	1.1200	.6100
		2	.6700	.6400
4376185	METHYL HYDROGEN PHTHALATE	1	.5800	.0310
19438109	METHYL 3-HYDROXYBENZOATE	1	.5500	.1600
		2	1.1250	.1000
99763	METHYLP-HYDROXYBENZOATE	2	1.3000	.1600
767599	METHYL-1-INDENE	1	.4900	.4400
		2	.3300	.4800
95205	2-METHYLINDOLE	1	.6800	.2000
		2	.7800	.2500
83341	3-METHYLINDOLE	1	.6800	.2900
		2	.7800	.4100
614960	5-METHYLINDOLE	1	.6300	.1200
7399497	1-METHYL-2-ISOPROPENYLBENZENE	1	.2800	.2200
535773	1-METHYL-3-ISOPROPYLBENZENE (M-CYMENE)	1	.3210	1.1200
		2	.1300	.7700
99876	1-METHYL-4-ISOPROPYLBENZENE	1	.3240	.8700
		2	.1500	.7000
111820	METHYL LAURATE	1	.7600	.9300
112630	METHYL LINOLEATE	1	1.4400	.2800
90120	1-METHYLNAPHTHALENE	1	.6300	.6200
		2	.4800	.5600
91576	2-METHYLNAPHTHALENE	1	.6100	.3200
		2	.4800	.3300
99558	2-METHYL-5-NITRO-ANILINE	1	.8000	.0670
111115	METHYL OCTANOATE	1	.4100	1.9500
		2	.1500	.7200
112629	METHYL OLEATE	1	1.3600	.0510

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** Relative to 2-fluorobiphenyl

GC Column Codes 1) 40 M SE-30 2) 50 M CARBOWAX 3) 25 M CP SIL-5

List of Standards

CASRN	Compound Name	GC	RRT*	RMR**
		2	.7900	.0920
107415	2-METHYL-2,4-PENTANEDIOL	1	.2200	.2000
		2	.3700	.1000
108101	4-METHYL-2-PENTANONE	1	.0920	.1500
		2	.0270	.1600
141797	4-METHYL-3-PENTEN-2-ONE	1	.1300	.2000
		2	.0620	.2500
832699	1-METHYLPHENANTHRENE	1	1.1400	.5100
		2	1.2100	.3400
2531842	2-METHYLPHENANTHRENE	1	1.1200	.8900
		2	1.1500	.4900
883205	9-METHYLPHENANTHRENE	1	1.1400	.4500
		2	1.2100	.3100
673325	METHYLPHENYLACETYLENE	1	.4000	.5500
		2	.2900	.5200
614006	METHYLPHENYLNITROSOAMINE	1	.3500	.1100
		2	.3400	.1100
1074175	1-METHYL-2-N-PROPYLBENZENE	1	.3670	.2700
		2	.1700	.8400
1074437	1-METHYL-3-N-PROPYLBENZENE	1	.3450	.7300
		2	.0789	.7200
2381217	1-METHYLPYRENE	1	1.6600	.7100
		3	1.5100	1.5200
3442782	2-METHYLPYRENE	1	1.6400	.1000
3353126	4-METHYLPYRENE	3	1.4900	.4500
109068	2-METHYLPYRIDINE	1	.1400	.1700
		2	.1100	.2000
112618	METHYL STEARATE	2	.7700	.5900
108996	3-METHYLPYRIDINE	1	.1700	.0960
		2	.1500	.1400
872504	N-METHYL-2-PYRROLIDINONE	1	.3500	.0420
		2	.3900	.1100

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** Relative to 2-fluorobiphenyl

GC Column Codes 1) 40 M SE-30 2) 50 M CARBOWAX 3) 25 M CP SIL-5

List of Standards

CASRN	Compound Name	GC	RRT*	RMR**
91634	2-METHYLQUINOLINE	1	.6300	.4300
		2	.5300	.6700
491350	4-METHYLQUINOLINE	1	.6700	.5400
		2	.6200	.5700
91623	6-METHYLQUINOLINE	1	.6500	.1600
		2	.5900	.3100
612602	7-METHYLQUINOLINE	1	.6500	.3000
		2	.5900	.3700
611325	8-METHYLQUINOLINE	1	.6300	.7500
		2	.5200	.7400
119368	METHYL SALICYLATE	1	.4700	.3400
112618	METHYL STEARATE	1	1.4100	.2700
98839	ALPHA-METHYLSTYRENE	1	.2500	.1800
		2	.1100	.1800
100801	M-METHYLSTYRENE	1	.3200	.1100
		2	.2000	.2200
611154	O-METHYLSTYRENE	1	.3300	.4800
		2	.2000	.2900
622979	P-METHYLSTYRENE	1	.3400	.3900
77418	METHYLSUXIMIDE	1	.8600	.1500
		2	.8800	.4400
124107	METHYL TETRADECANOATE(METHYL MYRISTATE)	1	.9100	1.1300
2809645	5-METHYLTETRALIN	1	.6200	.2200
		2	.3700	.3900
1073729	P-METHYLTHIOPHENOL	1	.6900	.0710
		2	1.0000	.0780
615225	2(METHYLTHIO)BENZOTHIAZOLE	1	.8300	.3800
		2	.7500	.2400
99752	METHYL P-TOLUATE	1	.4700	.0790
640619	N-METHYL-P-TOLUENESULFONAMIDE	1	.8800	.2600
		3	.8300	.1400

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** Relative to 2-fluorobiphenyl

GC Column Codes 1) 40 M SE-30 2) 50 M CARBOWAX 3) 25 M CP SIL-5

List of Standards

CASRN	Compound Name	GC	RRT*	RMR**
544638	MYRISTIC ACID	2	.9900	.0140
91203	NAPHTHALENE	1	.5100	.9100
		2	.4200	.8000
93094	2-NAPHTHOIC ACID	1	.9500	.0210
90153	1-NAPHTHOL	1	.7600	.2900
		2	1.2300	.0660
135193	2-NAPHTHOL	1	.6400	.2000
		2	1.3300	.0710
134327	1-NAPHTHYLAMINE	1	.7900	.2500
		2	.9600	.1000
142507	NEROLIDOL	1	.8000	.0040
54115	NICOTINE	1	.6600	.4400
		2	.4700	.7000
100016	P-NITROANILINE	1	.8400	.0130
91236	ORTHO-NITROANISOLE	1	.5700	.1100
98953	NITROBENZENE	1	.4000	.1400
		2	.4400	.1800
86000	2-NITROBIPHENYL	1	.9000	.0800
		2	.9300	.0700
2113588	3-NITROBIPHENYL	1	1.0300	.1500
119335	2-NITRO-P-CRESOL	2	.5000	.1200
6960425	7-NITROINDOLE	1	.8200	.0530
		2	1.0400	.0510
100298	P-NITROPHENETOLE	1	.7400	.0970
		2	.7000	.1200
88755	ORTHO-NITROPHENOL	2	.4600	.1000
100027	P-NITROPHENOL	1	.7500	.0099
586969	NITROSOBENZENE	1	.1730	.0830
88722	ORTHO-NITROTOLUENE	1	.4400	.2100

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** Relative to 2-fluorobiphenyl

GC Column Codes 1) 40 M SE-30 2) 50 M CARBOWAX 3) 25 M CP SIL-5

List of Standards

CASRN	Compound Name	GC	RRT*	RMR**
99990	PARA-NITROTOLUENE	1	.5000	.2400
		2	.4300	.2900
629925	NONADECANE	1	1.1100	.6000
		2	.5100	.9300
112050	NONANOIC ACID	1	.5600	.1400
		2	.5900	.0000
143088	1-NONANOL	1	.3800	.2500
104405	P-NONYLPHENOL	1	.9200	.0570
		2	.9500	.0500
76222	NORBORNAN-2-ONE (CAMPHOR)	1	.4800	.3300
		2	.2900	.2400
630024	N-OCTACOSANE	2	1.1500	.1800
		3	2.2100	.6600
593453	OCTADECANE	1	1.0100	.4900
		2	.4600	1.5000
112925	1-OCTADECANOL	1	1.3200	.2200
		2	.8700	.4000
112889	1-OCTADECENE	1	1.0000	.5300
		2	.5000	.2400
124072	OCTANOIC ACID	1	.3900	.1100
		2	.5600	.0700
111875	1-OCTANOL	1	.3400	.2500
111137	2-OCTANONE	1	.2700	.0580
		2	.0900	.0540
112801	OLEIC ACID	1	1.4300	.1700
		2	1.6400	.0420
57103	PALMITIC ACID	2	1.3700	.0039
123637	PARALDEHYDE	1	.0792	.4100
608935	PENTACHLOROBENZENE	1	.7900	.8100
		2	.5600	.6000
87865	PENTACHLOROPHENOL	1	.9800	.0660

* Retention data relative to D10ANTHRACENE
** Relative to 2-fluorobiphenyl

GC Column Codes 1) 40 M SE-30 2) 50 M CARBOWAX 3) 25 M CP SIL-5

List of Standards

CASRN	Compound Name	GC	RRT*	RMR**
		2	1.2500	.0270
		3	.9600	.3000
34774691	PENTACHLOROPROPENE	1	.3800	.3800
629992	N-PENTACOSANE	2	.8300	.4300
		3	1.6700	1.0800
629629	N-PENTADECANE	1	.7800	1.1600
		2	.2900	1.1400
700129	PENTAMETHYLBENZENE	1	.6100	.4200
		2	.3800	.4000
81038	1,1,3,3,5-PENTAMETHYL-2,3-DIHYDROINDENE	1	.5500	1.2700
109524	PENTANOIC ACID	2	.4000	.0900
107879	2-PENTANONE	1	.0460	.6400
76744	PENTOBARBITAL	1	.9800	.0078
538681	N-PENTYLBENZENE	1	.4900	.1500
		2	.2400	.3200
2719520	SEC-PENTYLBENZENE	1	.4200	.1100
		2	.1800	.1700
198550	PERYLENE	3	2.4000	1.1100
85018	PHENANTHRENE	1	.9900	.8400
		2	.9900	.5700
229878	PHENANTHRIDINE	1	1.0300	.2400
		2	1.2000	.2100
92820	PHENAZINE	1	.9500	.3700
		2	.9500	.2800
108952	PHENOL	1	.2300	.0720
		2	.5100	.3800
92842	PHENOTHIAZINE	1	1.3400	.0940
122598	PHENOXYACETIC ACID	2	.3750	.4200
3933946	4-PHENOXYBIPHENYL	1	1.4700	.3400
		3	1.4300	.7900
122996	2-PHENOXYETHANOL	1	.5200	.2600

* Retention data relative to D10ANTHRACENE
** Relative to 2-fluorobiphenyl

GC Column Codes 1) 40 M SE-30 2) 50 M CARBOWAX 3) 25 M CP SIL-5

List of Standards

CASRN	Compound Name	GC	RRT*	RMR**
		2	.6100	.4600
831823	P-PHENOXYPHENOL	1	.9500	.1100
		2	1.6100	.2900
103811	2-PHENYLACETAMIDE	1	.6900	.0270
		2	1.0000	.0840
122792	PHENYL ACETATE	1	.3400	.5200
		2	.2900	.5900
103822	PHENYLACETIC ACID	2	.9200	.0190
31017400	1-PHENYL-1-CYCLOHEXENE	1	.7000	.3400
		2	.4900	.2800
193395	2,3-O-PHENYLENEPYRENE	3	2.9700	.0330
98851	1-PHENYLETHANOL	1	.3800	.1500
		2	.4700	.2100
60128	2-PHENYL ETHANOL	1	.4200	.2800
		2	.5000	.5400
101848	PHENYL ETHER	1	.6900	.6200
		2	.5700	.5000
103719	PHENYL ISOCYANATE	1	.2900	.0890
605027	ALPHA-PHENYLNAPHTHALENE	1	1.0600	.4000
		2	.9200	.3400
612942	2-PHENYLNAPHTHALENE	1	1.1900	.4100
		2	1.2700	.3600
90302	N-PHENYL-1-NAPHTHYLENAMINE	1	1.4600	.1800
580518	M-PHENYLPHENOL	2	1.8500	.0610
90437	ORTHO-PHENYLPHENOL	1	.7700	.3300
		2	.8600	.1600
617947	2-PHENYL-2-PROPANOL(DIMETHYLBENZYL ALCOHOL)	1	.4200	.2600
		2	.4000	.2700
122974	3-PHENYLPROPANOL	1	.4800	.1300
300572	3-PHENYL-1-PROPENE (ALLYLBENZENE)	1	.2700	.2300
		2	.1200	.2400

* Retention data relative to D10ANTHRACENE
** Relative to 2-fluorobiphenyl

GC Column Codes 1) 40 M SE-30 2) 50 M CARBOWAX 3) 25 M CP SIL-5

List of Standards

CASRN	Compound Name	GC	RRT*	RMR**
501520	PHENYLPROPIONIC ACID (HYDROCINNAMIC ACID)	2	.9600	.0062
1459105	1-PHENYLTETRADECANE	1	1.3800	.6100
85449	PHTHALIC ANHYDRIDE	1	.6200	.0600
		3	.3800	.1000
87412	PHTHALIDE	1	.6400	.1100
		2	.7300	.2200
85416	PHTHALIMIDE	1	.7400	.0200
		2	1.2800	.0200
108894	GAMMA-PICOLINE	1	.1500	.1300
80568	ALPHA-PINENE	1	.3300	.5500
		2	.0620	.5300
18172673	BETA-PINENE	1	.2800	.6300
6752072	PIPERIDONE (DELTA-VALEROLACTAM)	1	.4300	.0150
89816	PIPERITONE	1	.5300	.3900
637503	PROPENYLBENZENE	1	.3600	.2400
		2	.2300	.1600
79094	PROPIONIC ACID	2	.3000	.0033
95636	1,2,4-TRIMETHYLBENZENE	1	.3200	.6800
93550	PROPIOPHENONE	1	.4700	.0740
95636	1,2,4-TRIMETHYLBENZENE	2	.1500	.5700
93550	PROPIOPHENONE	2	.4300	.0680
1569013	1-PROPOXYISOPROPANOL	1	.1500	.3500
		2	.0940	.3900
103651	N-PROPYLBENZENE	1	.2500	.9900
		2	.0990	.9700
645567	4-N-PROPYLPHENOL	2	.6500	.1500
129000	PYRENE	1	1.4000	.2100
110861	PYRIDINE	1	.0800	.0300

* Retention data relative to D10ANTHRACENE
** Relative to 2-fluorobiphenyl

GC Column Codes 1) 40 M SE-30 2) 50 M CARBOWAX 3) 25 M CP SIL-5

List of Standards

CASRN	Compound Name	GC	RRT*	RMR**
		2	.0780	.1100
109977	PYRROLE	1	.0800	.0300
		2	.2900	.0700
91225	QUINOLINE	1	.5600	.2400
		2	.5200	.4900
94597	SAFROLE	1	.6000	.3500
		2	.4700	.3300
90028	SALICYLALDEHYDE	1	.3800	.0750
		2	.4000	.0700
22328945	SECOBARBITAL	1	1.0800	.0540
		3	1.0200	.1200
122349	SIMAZINE	1	.9250	.1700
122394	DIPHENYLAMINE	1	.8200	.4600
7683649	SQUALENE	3	2.2200	.3100
57114	STEARIC ACID	1	1.4800	.0200
100425	STYRENE	1	.2000	.2600
		2	.1200	.2800
134963	SYRINGALDEHYDE	1	.8600	.1200
		2	1.3400	.0170
84151	O-TERPHENYL	1	1.0800	.9600
		2	.9200	.7000
623278	TEREPHTHALDEHYDE	1	.5300	.0540
		2	.5800	.1500
99865	ALPHA-TERPINENE	1	.3200	.3400
		2	.0450	.2400
99854	GAMMA-TERPINENE	1	.4100	.3900
		2	.1200	.2300
562743	TERPINENE-4-OL	1	.5100	.3600
		2	.3500	.2500
98555	ALPHA-TERPINEOL	1	.5100	.3700
		2	.4000	.2400
138874	BETA-TERPINEOL	1	.3600	.0560

* Retention data relative to D10ANTHRACENE
** Relative to 2-fluorobiphenyl

GC Column Codes 1) 40 M SE-30 2) 50 M CARBOWAX 3) 25 M CP SIL-5

List of Standards

CASRN	Compound Name	GC	RRT*	RMR**
586629	TERPINOLENE	1	.4200	.1500
		2	.1500	.1300
95943	1,2,4,5-TETRACHLOROBENZENE	1	.6200	.3100
		2	.2300	.6500
41464408	2,4,2',5'-TETRACHLOROBIPHENYL	1	1.1700	.1900
35693993	2,5,2',5'-TETRACHLOROBIPHENYL	1	1.1800	.2700
15968055	2,6,2',6'-TETRACHLOROBIPHENYL	1	1.0500	.3400
630206	1,1,1,2-TETRACHLOROETHANE	1	.1300	.2100
79345	1,1,2,2-TETRACHLOROETHANE	1	.2300	.2800
		2	.2700	.3400
127184	TETRACHLOROETHYLENE	1	.1400	.1600
		2	.0240	.2000
4901513	2,3,4,5-TETRACHLOROPHENOL	2	1.1900	.0100
58902	2,3,4,6-TETRACHLOROPHENOL	2	1.1600	.0038
935955	2,3,5,6-TETRACHLOROPHENOL	2	1.3100	.0020
629594	N-TETRADECANE	1	.7000	1.3800
		2	.2200	.8400
112721	TETRADECANOL	1	.8900	.2300
		2	.6000	.4600
1120361	TETRADECENE-1	1	.7000	.4200
		2	.2500	.2000
143248	TETRAETHYLENE GLYCOL DIMETHYL ETHER	1	.7600	1.1600
		2	.6000	1.5600
529340	ALPHA-TETRALONE	1	.6600	.1400
		2	.6100	.1500
488233	1,2,3,4-TETRAMETHYLBENZENE (PREHNITENE)	1	.4540	.8000
		2	.2600	.5400
527537	1,2,3,5-TETRAMETHYLBENZENE	1	.4230	.6300
		2	.2400	.3900
140669	P-(1,1,3,3-TETRAMETHYLBUTYL)PHENOL	2	.8600	.6500

* Retention data relative to D10ANTHRACENE
** Relative to 2-fluorobiphenyl

GC Column Codes 1) 40 M SE-30 2) 50 M CARBOWAX 3) 25 M CP SIL-5

List of Standards

CASRN	Compound Name	GC	RRT*	RMR**
941606	1,1,4,6-TETRAMETHYLINDAN	1	.6300	.1700
		2	.3500	.5200
942438	1,1,5,6-TETRAMETHYLINDAN	1	.6400	.2000
		2	.3400	.6100
75741	TETRAMETHYLLEAD	1	.0780	.3200
1921706	2,6,10,14-TETRAMETHYLPENTADECANE	1	.9200	1.2300
815247	2,2,4,4-TETRAMETHYL-3-PENTANONE	1	.2000	1.4500
492228	THIAXANTHONE(THIOXANTHEN-9-ONE)	1	1.3400	.0720
106456	P-THIOCRESOL	2	.3300	.0100
104870	P-TOLUALDEHYDE	1	.4000	.1800
		2	.3900	.1900
108883	TOLUENE	1	.1000	.2200
		2	.0280	.2100
88197	ORTHO-TOLUENESULFONAMIDE	1	.8600	.0100
		2	2.0400	.0082
70553	P-TOLUENESULPHONAMIDE	1	.8900	.0380
99047	M-TOLUIC ACID	2	.8500	.0210
118901	ORTHO-TOLUIC ACID	2	.8700	.0053
95534	ORTHO-TOLUIDINE	1	.4000	.2000
		2	.5000	.2900
638686	TRIACONTANE	2	1.5600	.0410
		3	2.5900	.8200
290879	S-TRIAZINE	1	.0630	.0940
		2	.0340	.2200
147820	2,4,6-TRIBROMOANILINE	1	.9000	.1700
78513	TRIBUTOXYETHYL PHOSPHATE	3	1.5200	3.7300
126738	TRIBUTYL PHOSPHATE	1	.8500	.4500
		2	.6000	2.0800
87616	1,2,3-TRICHLOROBENZENE	1	.5500	.2800

* Retention data relative to D10ANTHRACENE
** Relative to 2-fluorobiphenyl

GC Column Codes 1) 40 M SE-30 2) 50 M CARBOWAX 3) 25 M CP SIL-5

List of Standards

CASRN	Compound Name	GC	RRT*	RMR**
		2	.4200	.2100
120821	1,2,4-TRICHLOROBENZENE	1	.5100	.3500
		2	.3800	.3800
108703	1,3,5-TRICHLOROBENZENE	1	.4700	.3000
		2	.2800	.2700
55702460	2,3,4-TRICHLOROBIPHENYL	1	1.1100	.3000
15862074	2,4,5-TRICHLOROBIPHENYL	1	1.0500	.2900
38444814	2,5,3'-TRICHLOROBIPHENYL	1	1.0600	.2300
16606023	2,5,4'-TRICHLOROBIPHENYL	1	1.0700	.3600
38444869	3,4,2'-TRICHLOROBIPHENYL	1	1.1100	.3500
71556	1,1,1-TRICHLOROETHANE	1	.0530	.4000
79005	1,1,2-TRICHLOROETHANE	1	.1100	.1300
		2	.1100	.1300
79016	TRICHLOROETHYLENE	1	.0830	.2200
		2	.0300	.3000
933755	2,3,6-TRICHLOROPHENOL	1	.6400	.1900
		2	.8100	.0490
95954	2,4,5-TRICHLOROPHENOL	2	.7900	.0200
88062	2,4,6-TRICHLOROPHENOL	2	.6900	.1100
96184	1,2,3-TRICHLOROPROPANE	1	.2200	.2300
		2	.2600	.2000
6639301	2,4,5-TRICHLOROTOLUENE	1	.1400	.2400
		2	.4400	.2000
638675	N-TRICOSANE	1	1.8500	.6600
		2	.6600	1.2400
		3	1.5000	.5900
629505	N-TRIDECANE	1	.6200	1.2800
		2	.1500	.6100
638539	TRIDECANOIC ACID	2	.8800	.0580
593088	2-TRIDECANONE	1	.7300	1.0400

* Retention data relative to D10ANTHRACENE
** Relative to 2-fluorobiphenyl

GC Column Codes 1) 40 M SE-30 2) 50 M CARBOWAX 3) 25 M CP SIL-5

List of Standards

CASRN	Compound Name	GC	RRT*	RMR**
2437561	1-TRIDECENE	1	.6100	.3300
		2	.1900	.1300
102250	1,3,5-TRIETHYLBENZENE	1	.5000	.5800
112276	TRIETHYLENE GLYCOL	1	.5300	.7900
		2	.7100	.7600
143226	TRIETHYLENE GLYCOL N-BUTYL ETHER	1	.7400	.0600
		2	.6400	.2800
78400	TRIETHYL PHOSPHATE (ETHYL PHOSPHATE)	1	.4400	.3300
		2	.3600	.2900
717748	1,3,5-TRIISOPROPYLBENZENE	1	.6100	.9600
86817	3,4,5-TRIMETHOXYBENZALDEHYDE	1	.8200	.4000
		2	.8100	.2800
634366	1,2,3-TRIMETHOXYBENZENE	1	.5900	.4500
		2	.5200	.4100
1667012	2,4,6-TRIMETHYLACETOPHENONE	1	.6100	.1300
		2	.4900	.3000
526738	1,2,3-TRIMETHYLBENZENE	1	.2910	.6700
		2	.1700	.4800
108678	1,3,5-TRIMETHYLBENZENE(MESITYLENE)	1	.2650	.7200
		2	.1100	.6200
54340873	1,4,7-TRIMETHYLINDAN	1	.6300	.1900
		2	.3800	.3900
5711193	TRIMETHYLLEAD ACETATE	1	1.0100	.0000
2245387	2,3,5-TRIMETHYLNAPHTHALENE	1	.8300	.3800
		2	.6300	.6800
829265	2,3,6-TRIMETHYLNAPHTHALENE	1	.8200	.6600
		2	.5900	.5100
697825	2,3,5-TRIMETHYLPHENOL	2	.6100	.3300
496786	2,4,5-TRIMETHYLPHENOL	2	.6200	.3900
527606	2,4,6-TRIMETHYLPHENOL	1	.4900	.2800
		2	.5200	.3300

* Retention data relative to D10ANTHRACENE
** Relative to 2-fluorobiphenyl

GC Column Codes 1) 40 M SE-30 2) 50 M CARBOWAX 3) 25 M CP SIL-5

List of Standards

CASRN	Compound Name	GC	RRT*	RMR**
527548	3,4,5-TRIMETHYLPHENOL	1	.6000	.2200
		2	.6800	.2300
14667551	2,3,5-TRIMETHYLPYRAZINE	1	.3200	.5600
		2	.2100	.4700
1462846	2,3,6-TRIMETHYLPYRIDINE	1	.3300	.1600
		2	.2200	.1800
108758	2,4,6-TRIMETHYLPYRIDINE	1	.3200	.1300
		2	.2000	.3800
1806548	TRIOCTYL PHOSPHATE	3	1.6900	.7500
217594	TRIPHENYLENE	3	1.7000	.6600
115866	TRIPHENYL PHOSPHATE	3	1.5500	.2400
20324338	TRIPROPYLENE GLYCOL METHYL ETHER	1	.5900	.7600
		2	.4600	1.1300
291214	1,3,5-TRITHIANE	1	.5800	.0620
		2	.6100	.0790
3658808	2,3,4-TRITHIAPENTANE (DIMETHANE TRISULFIDE)	1	.2300	.0200
1120214	N-UNDECANE	1	.4300	.8000
		2	.0420	.0800
112378	UNDECANOIC ACID	2	.7300	.0700
112425	1-UNDECANOL	1	.6200	.3400
112129	2-UNDECANONE	1	.5700	1.1400
112389	UNDECYLENIC ACID (10-UNDECENOIC ACID)	2	.7600	.7000
121335	VANILLIN	1	.6700	.0890
		2	.8400	.0800
		3	.5000	.0110
93038	VERATRYL ALCOHOL	1	.7600	.0800
		2	.9100	.0900
105384	VINYLPROPIONATE	1	.0390	.0200
100696	2-VINYLPYRIDINE	1	.2700	.0890
		2	.2300	.1100

* Retention data relative to D10ANTHRACENE
** Relative to 2-fluorobiphenyl

GC Column Codes 1) 40 M SE-30 2) 50 M CARBOWAX 3) 25 M CP SIL-5

List of Standards

CASRN	Compound Name	GC	RRT*	RMR**
92831	XANTHENE	1	.8800	.5400
		2	.7800	.1600
90471	XANTHONE	1	1.0600	.1900
108383	M-XYLENE	1	.2100	.4100
		2	.0640	.3900
95476	ORTHO-XYLENE	1	.2200	.5600
		2	.0420	.1450
106423	P-XYLENE	1	.1900	.2500
		2	.0560	.2200
108689	3,5-XYLENOL	1	.4750	.1400
		2	.6000	.3000

* Retention data relative to D10ANTHRACENE
** Relative to 2-fluorobiphenyl

GC Column Codes 1) 40 M SE-30 2) 50 M CARBOWAX 3) 25 M CP SIL-5

Appendix B

List of Standards Not Available

CASRN	Compound Name
Status:	Standard was not eluted from column
506309	ARACHIDIC ACID(EICOSANOIC ACID)
67527	BARBITURIC ACID
79118	CHLOROACETIC ACID
86395	2-CHLORO-9H-THIOXANTHEN-9-ONE
57885	CHOLESTEROL*
26761400	DIISODECYL PHTHALATE
109875	DIMETHOXYMETHANE
84764	DINONYL PHTHALATE
119062	DITRIDECYL PHTHALATE
112856	DOCOSANOIC ACID
530574	4-HYDROXY-3,5-DIMETHOXYBENZOIC ACID
149304	2-MERCAPTOBENZOTHIAZOLE
1076228	3-METHYLXANTHINE
120183	2-NAPHTHALENE SULFONIC ACID
62237	P-NITROBENZOIC ACID
64040	BETA-PHENETHYLAMINE
88993	PHTHALIC ACID*
69727	SALICYLIC ACID*
142836	SORBALDEHYDE
7704349	SULFUR*
791286	TRIPHENYLPHOSPHINE OXIDE

*Compound Spectrum Identified in Extract; Methylene Chloride Solution Containing Compound Could Not be Chromatographed Successfully.

List of Standards Not Available

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   CASRN  Compound Name
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 Status:  In stock but not found in extract

11097691  AROCHLOR-1254-1 (TETRACHLOROBIPHENYL)
   77474  HEXACHLOROCYCLOPENTADIENE
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List of Standards Not Available

CASRN	Compound Name
Status:	Available commercially but too expensive to order
14315141	5-METHYL-2,3-BENZOTHIOPHENE
505102	3-METHYLTHIO-1-PROPANOL

List of Standards Not Available

CASRN	Compound Name
Status:	No commercial source
1587048	O-ALLYLTOLUENE
203123	2,13-BENZFLUORANTHENE
205823	10,11-BENZFLUORANTHENE
238846	1,2-BENZOFLUORENE
694871	BICYCLO(4.2.0)OCTA-1,3,5-TRIENE (BENZOCYCLOBUTANE)
6738041	2-BIPHENYLYL PHENYL ETHER
16536575	CIS-2-BROMOCYCLOHEXANOL
2917739	DI-N-BUTYL AZELATE
85701	BUTYL (BUTOXYCARBONYL)METHYL PHTHALATE
3913028	2-BUTYL-1-OCTANOL
577924	4-TERT-BUTYL-2-PHENYLPHENOL
7661394	2-N-BUTYLQUINOLINE
98282	2-CHLORO-4-TERT-BUTYLPHENOL
2441976	3-CHLOROCYCLOHEXENE
14862523	1-CHLORO-3,5-DIBROMOBENZENE
87649	3-CHLORO-2-HYDROXYTOLUENE (2-METHYL-6 CHLOROPHENOL)
39638329	BIS-(2-CHLOROISOPROPYL) ETHER
488971	CYCLOFENCHENE
19407284	DEHYDROABIETANE
54518046	DIBUTYL ORTHOFORMATE
13676589	1,4-DICHLOROBUTENE-1
2460493	4,5-DICHLOROGUAIACOL
4437223	DIFURFURYL ETHER
1197406	2,2-DIFURYLMETHANE
96480	DIHYDRO-2(3H)-FURANONE
2934056	2,4-DIISOPROPYLPHENOL
10375969	2,5-DIISOPROPYL-P-XYLENE
1738256	DIMETHYLAMINE PROPIONITRILE
5973717	3,4-DIMETHYLBENZALDEHYDE
16587409	2,7-DIMETHYLBENZO(B)THIOPHENE
1762272	DIMETHYLDIETHYLLEAD
1758889	1,4-DIMETHYL-2-ETHYLBENZENE
13360651	2,5-DIMETHYL-3-ETHYLPYRAZINE
1124352	2,4-DIMETHYL-6-ETHYLPYRIDINE
4612639	2,3-DIMETHYLFLUORENE
17057828	1,2-DIMETHYLINDAN
575371	1,7-DIMETHYLNAPHTHALENE
16587341	4,9-DIMETHYLNAPHTHO(2,3-B)THIOPHENE
3674655	2,3-DIMETHYLPHENANTHRENE
3674666	2,5-DIMETHYLPHENANTHRENE
3674699	4,5-DIMETHYLPHENANTHRENE
604831	9,10-DIMETHYLPHENANTHRENE
1195320	AR,ALPHA-DIMETHYLSTYRENE
16587501	3,6-DIMETHYL-1-THIAINDENE
2622675	1,2-DIPHENYLBENZIMIDAZOLE

List of Standards Not Available

CASRN	Compound Name
Status:	No commercial source
108576	M-DIVINYLBENZENE
17904277	EPIJUVABIONE
13925036	2-ETHYL-6-METHYLPYRAZINE
3999788	3-ETHYL-5-METHYLPYRIDINE
3710314	1,2-HEPTANEDIOL
2634335	3-HYDROXY-1,2-BENZISOTHIAZOLE
86771	2-HYDROXYDIBENZOFURAN
4899745	1-HYDROXY-3-(4-HYDROXY-3-METHOXYPHENYL)-2-PROPANONE
1687612	1-HYDROXY-3-METHYL-6-ETHYLBENZENE (3-METHYL-6-ETHYLPHENOL)
17465597	1,1,4,5,5,8-HEXAMETHYL-S-HYDRINDACENE
24614140	5-HYDROXY-2-METHYLPYRIMID-4-ONE
764896	8-HYDROXYOCTANOIC ACID
612204	ALPHA-HYDROXY-O-TOLUIC ACID
1135666	ISOLONGIFOLENE
1686664	ISOPIMARADIENE
4706892	1-ISOPROPYL-2,4-DIMETHYLBENZENE
4132723	1-ISOPROPYL-2,5-DIMETHYLBENZENE
4095221	2-ISOPROPYLTHIOPHENE
455163	4-METHYLBENZENESULFONYL FLUORIDE
2498773	1-METHYLBENZO(A)ANTHRACENE
4265252	2-METHYLBENZOFURAN
3652913	2-METHYLCARBAZOLE
4575466	1-METHYL-3-CYCLOHEXYLBENZENE
1235741	METHYL DEHYDROABIETATE
7320538	4-METHYLDIBENZO(BD)FURAN(4-METHYLDIPHENYLENE OXIDE)
16587523	3-METHYLDIBENZOTHIOPHENE
7372885	4-METHYLDIBENZOTHIOPHENE
767588	1-METHYL-(2,3-DIHYDROINDENE) (1-METHYLINDAN)
824635	2-METHYL-(2,3-DIHYDROINDENE) (2-METHYLINDAN)
824226	4-METHYL-(2,3-DIHYDROINDENE)(4-METHYLINDAN)
2717444	3-METHYL-1,2-DIHYDRONAPHTHALENE
2523377	9-METHYLFLUORENE
13129232	METHYL 3-FURUATE
777220	1-METHYLHEPTYLBENZENE
767602	3-METHYLINDENE
1761100	3-METHYLINDOLIZINE
3420028	6-METHYLINDOLE
1761111	6-METHYLINDOLIZINE
490653	1-METHYL-7-ISOPROPYLNAPHTHALENE
5129602	METHYL 14-METHYL PENTADECANDOATE (METHYL ISOPALMITATE)
13615402	3-METHYL-1-NAPHTHOL
20600571	2-METHYL-1-NAPHTHYL ISOCYANIDE
832713	3-METHYLPHENANTHRENE
33933732	2-METHYL-5-PROPYLTHIOPHENE
27587173	2-METHYLTEREPHTHALDEHYDE

List of Standards Not Available

CASRN	Compound Name
Status:	No commercial source
137064	ORTHO-METHYL THIOPHENOL
205436	NAPHTHOL(2,1-B)THIANAPHTHENE
239350	NAPHTHO(1,2-B)THIANAPHTHENE
1984049	1-NAPHTHYLISOCYANIDE
92933	4-NITROBIPHENYL
15619348	3-PHENYL-1,3-CYCLOHEXADIENE
4994165	4-PHENYLCYCLOHEXENE
931544	PHENYLISOCYANIDE
4534592	2-PHENYLTETRADECANE
1686562	SANDARACOPIMARADIENE
3387415	SABINENE
632213	1,1,3,3-TETRACHLORO-2-PROPANONE
54932784	P-(2,2,3,3-TETRAMETHYLBUTYL)PHENOL
28790865	2,3,4-TRIMETHYLCYCLOPENT-2-ENE-1-ONE
55682809	1,4,6-TRIMETHYL-1,2-DIHYDRONAPHTHALENE
17851273	2,4,5-TRIMETHYLETHYLBENZENE
1762261	TRIMETHYLETHYLLEAD
3302101	3,5,5-TRIMETHYLHEXANOIC ACID
40650417	1,1,5-TRIMETHYLINDANE
10222954	1,2,4-TRIMETHYL-5-ISOPROPYLBENZENE
3031081	1,3,6-TRIMETHYLNAPHTHALENE
3674735	2,3,5-TRIMETHYLPHENANTHRENE
3910358	1,1,3-TRIMETHYL-3-PHENYLINDAN
695987	2,3,5-TRIMETHYLPYRIDINE
289167	1,2,4-TRITHIOLANE
1453061	4-(2,5-XYLYL)BUTANOIC ACID

Appendix C

IC CODE	INDUSTRIAL CATEGORY	NO. OF EXTRACTS	%
1	TIMBER PRODUCTS	30	6.19
2	STEAM ELECTRIC	3	.62
3	LEATHER TANNING	5	1.03
4	IRON & STEEL MFG.	7	1.44
5	PETROLEUM REFINING	21	4.33
6	NONFERROUS METALS	15	3.09
8	PAINT & INK	27	5.57
9	PRINTING & PUBLISHING	8	1.65
10	ORE MINING	7	1.44
11	COAL MINING	10	2.06
12	ORGANICS & PLASTICS	49	10.10
13	INORGANIC CHEMICALS	15	3.09
14	TEXTILE MILLS	9	1.86
15	PLASTICS & SYNTHETICS	4	.82
16	PULP & PAPER	32	6.60
17	RUBBER PROCESSING	18	3.71
18	SOAPS & DETERGENTS	4	.82
19	AUTO & OTHER LAUNDRIES	23	4.74
20	PESTICIDES MFG.	8	1.65
21	PHOTOGRAPHIC INDUSTRIES	8	1.65
23	PHARMACEUTICALS	7	1.44
24	EXPLOSIVES	1	.21
27	PLASTICS MFG.	6	1.24
28	FOUNDRIES	2	.41
30	PORCELAIN/ENAMELING	1	.21
33	ELECTRONICS	32	6.60
36	OIL AND GAS EXTRACTION	3	.62
39	ORGANIC CHEMICALS	31	6.39
40	MECHANICAL PRODUCTS	26	5.36
41	TRANSPORTATION EQUIPMENT	6	1.24
42	AMUSEMENTS&ATHLETIC GOODS	7	1.44
44	SYNFUELS	2	.41
50	PUBLIC OWNED TREAT WORKS	44	9.07
98	INDUSTRY UNKNOWN	4	.82
99	RUM INDUSTRY	10	2.06

Appendix D

Confirmed Compounds
Sorted by CASRN

CASRN	Compound Name	# of occurrences of compound	IC's
50328	3,4-BENZPYRENE	1	50
51445	3,4-DICHLOROBENZOIC ACID	2	19,19
54115	NICOTINE	3	16,19,40
56553	1,2-BENZANTHRACENE	3	01,04,40
57103	PALMITIC ACID	7	08,09,14, 40,50,50, 98
57114	STEARIC ACID	2	16,50
57885	CHOLESTEROL	1	14
58082	CAFFEINE	7	16,19,40, 50,50,50, 98
58902	2,3,4,6-TETRACHLOROPHENOL	5	08,12,33, 40,42
59507	4-CHLORO-M-CRESOL	2	40,41
60093	4-AMINO-AZOBENZENE	1	12
60128	2-PHENYL ETHANOL	4	01,12,44, 99
60571	DIELDRIN	1	50
62533	ANILINE	4	01,12,17, 50

Confirmed Compounds
Sorted by CASRN

CASRN	Compound Name	# of occurrences of compound	IC's
64197	ETHANOIC ACID (ACETIC ACID)	1	39
65850	BENZOIC ACID	11	01,06,08, 09,10,14, 15,16,33, 40,41
67663	CHLOROFORM	1	12
67685	DIMETHYL SULPHOXIDE	1	16
67710	DIMETHYL SULFONE	3	16,16,33
67721	HEXACHLOROETHANE	1	39
68122	N,N-DIMETHYLFORMAMIDE	1	12
69727	SALICYLIC ACID	2	01,12
70553	P-TOLUENESULPHONAMIDE	2	06,09
71363	1-BUTANOL	1	13
71432	BENZENE	6	01,06,08, 09,17,33
71556	1,1,1-TRICHLOROETHANE	1	16
75741	TETRAMETHYLLEAD	1	06
76222	NORBORNAN-2-ONE (CAMPHOR)	4	01,08,14, 40

Confirmed Compounds
Sorted by CASRN

CASRN	Compound Name	# of occurrences of compound	IC's
78400	TRIETHYL PHOSPHATE (ETHYL PHOSPHATE)	1	50
78591	3,5,5-TRIMETHYL-2-CYCLOHEXENONE(ISOPHORONE)	2	08,16
79005	1,1,2-TRICHLOROETHANE	1	41
79016	TRICHLOROETHYLENE	2	19,41
79094	PROPANOIC ACID(PROPIONIC ACID)	2	14,50
79312	ISOBUTYRIC ACID	4	08,14,19,39
79414	METHACRYLIC ACID	1	08
79925	CAMPHENE	1	17
80568	ALFA-PINENE	1	16
82053	BENZANTHRONE	1	12
83329	ACENAPHTHENE	4	01,05,39,50
83330	1-INDANONE	3	17,33,50
83341	3-METHYLINDOLE	2	23,50
84651	9,10-ANTHRAQUINONE	2	01,12
84662	DIETHYL PHTHALATE	4	12,13,16,50

Confirmed Compounds
Sorted by CASRN

CASRN	Compound Name	# of occurrences of compound	IC's
84695	DIISOBUTYL PHTHALATE	1	02
84742	BUTYL PHTHALATE	12	02,06,08, 09,12,16, 16,19,33, 39,39,50
84764	DINONYL PHTHALATE	1	06
85018	PHENANTHRENE	9	01,04,05, 06,08,11, 16,33,39
85687	BUTYL BENZYL PHTHALATE	4	06,12,16, 28
86737	FLUORENE	5	01,05,11, 12,39
86748	CARBAZOLE	3	01,19,50
86817	3,4,5-TRIMETHOXYBENZALDEHYDE	1	16
87412	PHTHALIDE	1	15
87616	1,2,3-TRICHLOROBENZENE	4	14,33,39, 50
87650	2,6-DICHLOROPHENOL	1	33
87865	PENTACHLOROPHENOL	1	12
88062	2,4,6-TRICHLOROPHENOL	4	10,12,20, 39

Confirmed Compounds
Sorted by CASRN

CASRN	Compound Name	# of occurrences of compound	IC's
88697	ORTHO-ISOPROPYLPHENOL (ORTHO-CUMENOL)	3	04,17,50
88722	ORTHO-NITROTOLUENE	1	13
88755	ORTHO-NITROPHENOL	2	21,33
88993	PHTHALIC ACID	1	15
89634	4-CHLORO-2-NITROANILINE	1	12
89816	PIPERITONE	1	16
89952	O-METHYLBENZYL ALCOHOL	1	08
90006	O-ETHYLPHENOL	3	05,33,50
90028	SALICYLALDEHYDE	1	12
90051	O-METHOXYPHENOL	5	01,03,12, 16,99
90120	1-METHYL NAPHTHALENE	18	01,01,03, 04,05,06, 08,09,10, 11,12,16, 19,33,39, 40,42,50
90131	1-CHLORONAPTHALENE	2	50,50
90153	1-NAPHTHOL	1	09
90302	1-Naphthalenamine,N-phenyl-	1	06

Confirmed Compounds
Sorted by CASRN

CASRN	Compound Name	# of occurrences of compound	IC's
90437	1-HYDROXY-2-PHENYLBENZENE	7	04,12,13, 23,33,40, 50
91167	1,2-DIMETHOXYBENZENE (VERATROLE)	1	16
91203	NAPHTHALENE	23	01,01,03, 04,05,06, 08,10,11, 12,13,16, 17,19,24, 28,33,36, 39,40,41, 42,50
91225	QUINOLINE (1-BENZAZINE)	4	01,04,17, 50
91576	2-METHYLNAPHTHALENE	19	01,01,03, 04,04,05, 06,08,10, 11,13,16, 19,33,36, 39,40,42, 50
91598	2-AMINONAPHTHALENE	1	09
92524	BIPHENYL	8	01,12,12, 14,15,18, 39,98
92842	PHENOTHIAZINE	2	12,17
93550	PROPIOPHENONE	1	39
93583	METHYL BENZOATE	2	12,39

Confirmed Compounds
Sorted by CASRN

CASRN	Compound Name	# of occurrences of compound	IC's
93981	BENZANILIDE	1	09
94597	SAFROLE	4	03,21,40,41
95136	INDENE	1	01
95158	2,3-BENZOTHIOPENE (THIANAPHTHENE)	2	01,05
95169	BENZOTHIAZOLE	8	17,20,21,30,33,33,40,40
95205	2-METHYLINDOLE	2	05,50
95476	1,2-DIMETHYLBENZENE(O-XYLENE)	14	05,08,09,13,16,17,19,20,23,33,39,40,42,50
95487	ORTHO-CRESOL (2-METHYLPHENOL)	10	01,04,11,12,12,13,14,15,39,50
95498	O-CHLOROTOLUENE	3	12,39,98
95501	O-DICHLOROBENZENE	6	03,12,13,33,39,50
95512	2-CHLOROANILINE	1	39
95534	O-TOLUIDINE	3	09,13,50

Confirmed Compounds
Sorted by CASRN

CASRN	Compound Name	# of occurrences of compound	IC's
95567	O-BROMOPHENOL	1	21
95578	O-CHLOROPHENOL	2	13,39
95636	1,2,4-TRIMETHYLBENZENE	14	01,04,05, 08,09,10, 13,14,19, 27,33,39, 40,50
95738	2,4-DICHLOROTOLUENE	1	17
95750	3,4-DICHLOROTOLUENE	1	17
95761	3,4-DICHLOROANILINE	2	12,50
95874	1-HYDROXY-2,5-DIMETHYLBENZENE(2,5-DIMETHYLPHENOL	2	05,50
95932	1,2,4,5-TETRAMETHYLBENZENE	5	17,19,27, 33,50
95943	1,2,4,5-TETRACHLOROBENZENE	1	39
95954	2,4,5-TRICHLOROPHENOL	5	03,12,13, 16,33
96093	EPOXYETHYL BENZENE (STYRENE OXIDE)	1	17
96764	2,4-DI-TERT-BUTYLPHENOL	2	50,50
97530	EUGENOL	1	16
97541	2-METHOXY-4-(PROP-2-ENYL)-PHENOL (ISOEUGENOL)	1	16

Confirmed Compounds
Sorted by CASRN

CASRN	Compound Name	# of occurrences of compound	IC's
98000	FURFURYL ALCOHOL	4	16,44,50,99
98011	2-FURALDEHYDE	5	01,16,24,33,99
98544	P-TERT-BUTYLPHENOL (IN METHANOL)	6	12,17,33,39,40,50
98555	ALPHA-TERPINEOL	16	01,03,08,08,13,16,17,19,33,33,40,40,40,42,50,98
98737	P-TERT-BUTYLBENZOIC ACID	3	05,08,33
98828	ISOPROPYLBENZENE	9	05,08,13,14,17,27,40,50,50
98836	ALPHA-METHYLSTYRENE	1	09
98851	1-PHENYLETHANOL	1	40
98862	ACETOPHENONE	7	08,09,16,33,39,40,41
98953	Benzene,nitro-	5	12,12,12,12,13
99036	M-AMINOACETOPHENONE	1	39

Confirmed Compounds
Sorted by CASRN

CASRN	Compound Name	# of occurrences of compound	IC's
99047	M-TOLUIC ACID	6	08,14,15, 33,40,50
99309	2,6-DICHLORO-4-NITROANILINE	1	12
99627	1,3-DIISOPROPYLBENZENE	1	39
99650	1,3-DINITROBENZENE	1	12
99752	P-TOLUIC ACID,METHYL ESTER	1	39
99865	ALPHA TERPINENE	1	50
99876	P-CYMENE	9	04,05,06, 11,16,17, 19,33,40
99898	P-ISOPROPYLPHENOL	2	08,50
99990	PARA-NITROTOLUENE	1	13
100016	P-NITROANILINE	1	12
100185	P-DIISOPROPYLBENZENE	1	39
100414	ETHYLBENZENE	15	01,05,08, 13,14,15, 16,17,19, 33,39,39, 40,42,50
100425	STYRENE	9	08,12,12, 13,16,17, 17,19,19

Confirmed Compounds
Sorted by CASRN

CASRN	Compound Name	# of occurrences of compound	IC's
100470	BENZONITRILE (CYANOBENZENE)	2	01,39
100516	BENZYL ALCOHOL	10	05,06,08, 12,16,39, 39,50,98, 99
100527	BENZALDEHYDE	2	06,12
100696	2-VINYLPYRIDINE	2	17,50
100710	2-ETHYLPYRIDINE	1	17
101815	DIPHENYLMETHANE	3	12,23,39
101848	DIPHENYLETHER	9	12,12,15, 17,18,18, 33,39,98
103333	AZOBENZENE	1	19
103491	DIBENZYLAMINE	1	19
103651	N-PROPYLBENZENE	6	05,14,19, 27,27,50
103811	2-PHENYLACETAMIDE	1	39
103822	PHENYLACETIC ACID	10	04,12,12, 14,16,23, 33,39,40, 50
104405	P-NONYLPHENOL	2	06,39

Confirmed Compounds
Sorted by CASRN

CASRN	Compound Name	# of occurrences of compound	IC's
104767	2-ETHYL-1-HEXANOL	14	01,06,08, 08,08,09, 12,14,14, 17,33,39, 42,99
104905	2-METHYL-5-ETHYLPYRIDINE	1	39
104949	4-METHOXYANILINE	1	12
105135	P-ANISYLALCOHOL	1	01
105679	2,4-XYLENOL	6	04,05,12, 17,39,50
106332	ETHYL LAURATE	2	18,18
106412	P-BROMOPHENOL	1	21
106423	1,4-DIMETHYLBENZENE(P-XYLENE)	17	02,05,06, 08,09,10, 11,13,14, 21,23,27, 33,39,40, 42,50
106445	P-CRESOL	10	01,03,12, 14,17,19, 33,40,44, 50
106467	1,4-DICHLOROBENZENE	5	12,13,33, 39,50
106489	P-CHLOROPHENOL	1	12

Confirmed Compounds
Sorted by CASRN

CASRN	Compound Name	# of occurrences of compound	IC's
106934	1,2-DIBROMOETHANE	1	50
107142	CHLOROETHANENITRILE(CHLOROACETONITRILE)	1	33
107415	2-METHYL-2,4-PENTANEDIOL	5	04,06,08,14,40
107926	N-BUTANOIC ACID(BUTYRIC ACID)	7	01,03,09,14,19,42,50
108101	4-METHYL-2-PENTANONE	5	09,11,27,33,39
108372	1-BROMO-3-CHLOROBENZENE	1	39
108383	1,3-DIMETHYLBENZENE(M-XYLENE)	17	01,05,06,08,10,11,12,13,14,17,19,27,33,39,40,42,50
108394	META-CRESOL (3-METHYLPHENOL)	12	01,03,04,05,08,12,14,19,21,23,50,50
108429	M-CHLOROANILINE	2	12,23
108430	M-CHLOROPHENOL	1	12
108509	2,6-DIMETHYLPYRAZINE	1	99
108678	1,3,5-TRIMETHYLBENZENE	9	05,08,10,13,14,19,27,33,50

Confirmed Compounds
Sorted by CASRN

CASRN	Compound Name	# of occurrences of compound	IC's
108689	3,5-DIMETHYL PHENOL	6	01,05,11, 17,39,50
108703	1,3,5-TRICHLOROBENZENE	1	50
108758	2,4,6-TRIMETHYL PYRIDINE	1	01
108883	METHYLBENZENE (TOLUENE)	14	03,05,12, 13,13,17, 19,23,27, 33,39,40, 41,50
108907	CHLOROBENZENE	1	39
108941	CYCLOHEXANONE	1	08
108952	PHENOL	19	01,03,04, 05,06,08, 12,14,15, 16,19,21, 28,33,39, 40,44,50, 99
108985	BENZENETHIOL (THIOPHENOL)	1	05
109068	2-METHYLPYRIDINE	2	01,50
109524	VALERIC ACID	10	03,08,09, 12,14,16, 33,36,40, 50
110429	METHYL CAPRATE	1	18

Confirmed Compounds
Sorted by CASRN

CASRN	Compound Name	# of occurrences of compound	IC's
110430	HEPTAN-2-ONE	2	08,33
110656	BUTYNE-1,4-DIOL	1	12
110805	2-ETHOXYETHANOL (ETHYLENE GLYCOL MONOETHYL ETHER	1	33
110838	CYCLOHEXENE	2	33,99
110861	PYRIDINE	2	01,13
111115	OCTANOIC ACID-METHYL ESTER	1	18
111148	HEPTANOIC ACID	5	10,12,19, 40,50
111444	BIS(2-CHLOROETHYL)ETHER	1	20
111762	2-N-BUTOXYETHANOL	11	08,09,14, 16,17,19, 33,39,41, 42,50
111773	2-(2-METHOXYETHOXY)ETHANOL	1	08
111820	METHYL LAURATE	1	18
111900	2-(2-ETHOXYETHOXY) ETHANOL	5	04,09,16, 42,50
112050	NONANOIC ACID	7	10,19,30, 33,33,40, 50

Confirmed Compounds
Sorted by CASRN

CASRN	Compound Name	# of occurrences of compound	IC's
112129	2-UNDECANONE	2	18,18
112254	2-HEXYLOXYETHANOL	2	33,41
112345	2-(2-BUTOXYETHOXY) ETHANOL	24	01,05,08, 09,11,12, 12,13,14, 14,15,16, 17,17,19, 19,21,28, 33,42,50, 98,98,99
112390	METHYL HEXADECANOATE	5	01,04,06, 12,42
112403	N-DODECANE	15	01,04,05, 06,08,08, 09,10,11, 14,19,33, 39,42,50
112425	1-UNDECANOL	1	39
112538	DODECANOL	2	06,14
112618	STEARIC ACID METHYL ESTER	4	06,18,19, 40
112629	METHYL OLEATE	1	06
112630	METHYL LINOLEATE	1	23
112721	TETRADECANOL	3	09,14,50

Confirmed Compounds
Sorted by CASRN

CASRN	Compound Name	# of occurrences of compound	IC's
112925	1-OCTADECANOL	2	12,14
112958	N-EICOSANE	13	01,05,06, 08,09,11, 13,16,19, 33,39,40, 50
115195	2-METHYL-3-BUTYN-2-OL	1	33
115866	TRI-PHENYL PHOSPHATE	2	06,40
117817	DI-(2-ETHYLHEXYL)PHTHALATE	13	02,11,12, 12,12,15, 16,17,20, 28,50,50, 98
117840	DIOCTYL PHTHALATE	4	06,12,12, 39
118901	O-TOLUIC ACID	3	08,33,39
118934	O-HYDROXYACETOPHENONE	1	20
119335	2-NITRO-P-CRESOL	2	21,39
119619	BENZOPHENONE	3	08,23,40
119653	ISOQUINOLINE	1	01
120127	ANTHRACENE	12	01,04,05, 06,11,12, 16,19,24, 33,39,50

Confirmed Compounds
Sorted by CASRN

CASRN	Compound Name	# of occurrences of compound	IC's
120616	DIMETHYLTEREPHTHALATE	2	12,39
120729	INDOLE	6	01,03,04, 12,44,50
120752	2-METHYLBENZOTHIAZOLE	1	17
120821	1,2,4 TRICHLOROBENZENE	4	09,14,33, 39
120832	2,4-DICHLOROPHENOL	4	12,16,20, 39
121142	2,4-DINITROTOLUENE	1	13
121335	VANILLIN (4-HYDROXY-3-METHOXY BENZALDEHYDE)	7	01,03,06, 12,13,16, 33
121733	1-CHLORO-3-NITROBENZENE	1	12
122394	DIPHENYLAMINE	4	12,13,17, 17
122974	3-PHENYLPROPANOL	2	01,99
122996	2-PHENOXYETHANOL	4	08,12,21, 40
123079	P-ETHYLPHENOL	7	01,04,05, 12,17,40, 50
123080	P-HYDROXY-BENZALDEHYDE	1	12

Confirmed Compounds
Sorted by CASRN

CASRN	Compound Name	# of occurrences of compound	IC's
123422	2-HYDROXY-2-METHYL-4-PENTANONE (DIACETONE)	2	12,17
123513	3-METHYL-1-BUTANOL	1	44
123637	PARALDEHYDE	1	50
123795	DIOCTYL ADIPATE	1	16
123911	1,4-DIOXANE	2	39,50
124061	ETHYL MYRISTATE	2	18,99
124072	CAPRYLIC ACID	11	08,09,10, 12,12,16, 17,19,33, 40,50
124107	METHYL TETRADECANOATE	2	18,42
124185	N-DECANE	10	05,09,10, 12,14,19, 20,33,40, 50
126738	TRI-BUTYL PHOSPHATE	5	08,08,09, 12,16
127184	TETRACHLOROETHYLENE	17	01,03,05, 06,08,09, 11,12,15, 16,17,18, 20,41,50, 50,98
128370	(2,6-DI-TERT-BUTYL-4-METHYL PHENOL)	8	05,10,11, 13,15,17, 21,39

Confirmed Compounds
Sorted by CASRN

CASRN	Compound Name	# of occurrences of compound	IC's
129000	PYRENE (BENZOPHENANTHRENE)	7	04,06,12, 12,16,40, 50
131113	DIMETHYL PHTHALATE	2	08,12
132649	DIBENZOFURAN	4	01,04,11, 50
132650	DIBENZOTHIOPHENE	5	01,01,05, 06,16
134963	SYRINGALDEHYDE	3	01,12,16
135013	1,2-DIETHYLBENZENE	2	08,40
135193	2-NAPHTHOL	2	01,09
135988	SEC-BUTYLBENZENE	6	10,11,13, 14,19,33
138863	LIMONENE	3	03,12,17
139662	DIPHENYL SULFIDE	1	39
140114	BENZYL ACETATE	1	12
140670	P-ALLYLANISOLE	1	16
141797	4-METHYL-3-PENTEN-2-ONE	1	39
141935	M-DIETHYLBENZENE	5	08,14,19, 27,39

Confirmed Compounds
Sorted by CASRN

CASRN	Compound Name	# of occurrences of compound	IC's
142507	NEROLIDOL	1	16
142621	HEXANOIC ACID(CAPROIC ACID)	11	08,10,12, 12,16,17, 19,21,33, 40,50
143077	LAURIC ACID	11	08,12,14, 16,18,19, 20,23,30, 42,50
143226	TRIETHYLENE GLYCOL N-BUTYL ETHER	3	08,09,39
143248	TETRAETHYLENE GLYCOL DIMETHYL ETHER	1	08
147477	2,2,4-TRIMETHYLDIHYDROQUINOLINE	2	17,17
147820	2,4,6-TRIBROMOANILINE	1	17
150765	P-METHOXYPHENOL	1	16
150787	P-DIMETHOXYBENZENE	1	06
198550	PERYLENE	1	01
203645	4,5-METHYLENE PHENANTHRENE	2	01,12
206440	FLUORANTHENE (1,2-BENZACENAPTHENE)	5	01,04,06, 12,50
207089	BENZO(K)FLUORANTHENE	2	01,04

Confirmed Compounds
Sorted by CASRN

CASRN	Compound Name	# of occurrences of compound	IC's
208968	ACENAPHTHALENE	2	01,04
217594	TRIPHENYLENE	1	01
218019	CHRYSENE	3	01,04,50
243174	2,3 BENZOFLUORENE	2	01,11
259790	BIPHENYLENE	3	01,12,39
271896	BENZOFURAN	1	01
291214	1,3,5-TRITHIANE	1	03
300572	3-PHENYL-1-PROPENE (ALLYLBENZENE)	1	17
306081	4-HYDROXY-3-METHOXY-PHENYLACETIC ACID	2	01,16
334485	DECANOIC ACID	8	08,10,12, 16,18,19, 33,50
367124	O-FLUOROPHENOL	1	33
470826	1,8-CINEOLE	1	17
475207	LONGIFOLENE	1	50
486259	FLUORENONE	1	13
488233	1,2,3,4-TETRAMETHYLBENZENE (PREHNITENE)	7	08,10,17, 19,33,33, 42

Confirmed Compounds
Sorted by CASRN

CASRN	Compound Name	# of occurrences of compound	IC's
492228	THIAXANTHONE	1	23
496117	2,3-DIHYDROINDENE	4	01,05,19, 39
496162	2,3-DIHYDROBENZOFURAN	1	99
496786	2,4,5-TRIMETHYLPHENOL	2	01,50
498022	ACETOVANILLON (4-HYDROXY-3-METHOXYACETOPHENONE)	5	01,12,13, 16,99
499069	3,5-DIMETHYL-BENZOIC ACID	1	50
499752	CARVACROL (2-HYDROXY-4-ISOPROPYL-1-METHYLBENZENE	3	12,16,23
501520	PHENYLPROPIONIC ACID	5	01,06,12, 16,23
504201	2,6-DIMETHYL-2,5-HEPTADIEN-4-ONE	1	39
507700	BORNEOL	8	08,13,14, 16,16,17, 33,40
526738	1,2,3-TRIMETHYLBENZENE	15	01,01,04, 05,08,09, 10,13,14, 14,19,27, 39,40,50
526750	2,3-DIMETHYLPHENOL	3	01,05,50
527537	1,2,3,5-TETRAMETHYLBENZENE	3	17,19,33

Confirmed Compounds
Sorted by CASRN

CASRN	Compound Name	# of occurrences of compound	IC's
527548	3,4,5-TRIMETHYLPHENOL	1	50
527606	2,4,6-TRIMETHYLPHENOL	2	05,50
527844	1-METHYL-2-ISOPROPYLBENZENE	5	05,11,14, 19,33
529340	1-TETRALONE	3	12,13,39
535773	1-METHYL-3-ISOPROPYLBENZENE	8	04,05,06, 16,19,39, 42,50
535808	M-CHLOROBENZOIC ACID	1	16
540385	P-IODOPHENOL	1	33
541731	1,3-DICHLOROBENZENE	3	03,33,50
544638	MYRISTIC ACID	7	08,09,14, 33,42,50, 50
544763	N-HEXADECANE	20	01,02,04, 05,06,08, 09,10,11, 16,17,19, 21,33,33, 39,40,41, 42,50
554007	2,4-DICHLOROANILINE	1	39
562743	TERPINENE-4-OL	2	16,16

Confirmed Compounds
Sorted by CASRN

CASRN	Compound Name	# of occurrences of compound	IC's
569415	1,8-DIMETHYLNAPHTHALENE	1	40
571584	1,4-DIMETHYLNAPHTHALENE	9	01,05,06,19,33,39,40,42,50
571619	1,5-DIMETHYLNAPHTHALENE	13	01,04,05,06,08,09,10,11,16,19,33,40,42
573988	Naphthalene,1,2-dimethyl-	2	12,36
575417	1,3-DIMETHYLNAPHTHALENE	14	04,05,06,08,08,10,11,19,33,36,39,40,42,50
575439	1,6-DIMETHYLNAPHTHALENE	11	04,05,10,11,12,19,33,36,39,40,50
576261	2,6-DIMETHYL PHENOL	4	05,11,12,50
581408	2,3-DIMETHYLNAPHTHALENE	3	05,40,50
581420	2,6-DIMETHYLNAPHTHALENE	3	01,05,11
582161	2,7-DIMETHYLNAPHTHALENE	15	01,03,04,05,08,09,10,11,13,20,33,36,40,42,50

Confirmed Compounds
Sorted by CASRN

CASRN	Compound Name	# of occurrences of compound	IC's
585342	M-TERT-BUTYLPHENOL	1	33
586629	TERPINOLENE	1	16
589924	4-METHYLCYCLOHEXANONE	1	12
593088	2-TRIDECANONE	2	18,18
593453	OCTADECANE	16	01,02,04,05,06,08,09,11,16,17,19,21,33,39,40,50
593497	N-HEPTACOSANE	3	01,05,16
605027	Naphthalene,1-phenyl-	2	01,40
606202	2,6-DINITROTOLUENE	1	13
608275	2,3-DICHLOROANILINE	1	39
610720	2,5-DIMETHYL-BENZOIC ACID	1	33
611018	2,4-DIMETHYL-BENZOIC ACID	1	33
611143	1-METHYL-2-ETHYLBENZENE	16	04,05,08,10,11,13,13,14,17,19,27,33,39,40,42,50

Confirmed Compounds
Sorted by CASRN

CASRN	Compound Name	# of occurrences of compound	IC's
611154	O-METHYLSTYRENE	3	13,27,39
612000	1,1-DIPHENYLETHANE	1	12
612942	2-PHENYLNAPHTHALENE	2	01,01
613127	2-METHYL ANTHRACENE	4	05,06,11, 50
614006	METHYLPHENYLNITROSOAMINE	1	39
614960	5-METHYLINDOLE	1	50
615225	2(METHYLTHIO)BENZOTHIAZOLE	2	16,17
616239	2,3-DICHLORO-1-PROPANOL	1	11
617947	2-PHENYL-2-PROPANOL	2	12,41
618451	META-ISOPROPYLPHENOL	1	01
619045	3,4-DIMETHYL-BENZOIC ACID	3	33,39,50
620144	1-METHYL-3-ETHYLBENZENE	15	05,08,09, 10,11,12, 13,14,17, 19,27,33, 39,40,50
620177	META-ETHYLPHENOL	3	05,39,50
621829	CINNAMIC ACID	1	01

Confirmed Compounds
Sorted by CASRN

CASRN	Compound Name	# of occurrences of compound	IC's
622968	P-ETHYLTOLUENE	15	04,05,08,10,11,13,14,16,17,17,27,33,39,50,50
624920	DIMETHYLDISULFIDE	2	16,50
628977	ETHYL PALMITATE	1	99
629505	TRIDECANE	14	01,04,05,06,08,09,11,16,19,33,39,40,42,50
629594	N-TETRADECANE	17	01,04,05,06,08,08,10,11,13,16,18,19,33,39,40,42,50
629629	PENTADECANE	17	01,02,05,06,08,08,09,10,11,16,17,18,19,33,39,40,50
629732	1-HEXADECENE	1	14
629787	N-HEPTADECANE	14	02,04,05,06,08,08,09,16,17,19,33,40,41,50

Confirmed Compounds
Sorted by CASRN

CASRN	Compound Name	# of occurrences of compound	IC's
629925	NONADECANE	11	01,04,05, 06,08,09, 11,19,33, 40,50
629947	N-HENEICOSANE	1	05
629970	N-DOCOSANE	2	01,05
629992	N-PENTACOSANE	6	05,14,16, 19,33,40
630013	N-HEXACOSANE	3	05,19,33
630024	N-OCTACOSANE	1	05
630206	1,1,1,2-TETRACHLOROETHANE	1	33
634366	1,2,3-TRIMETHOXYBENZENE	1	16
637503	PROPENYLBENZENE	1	12
638539	TRIDECANOIC ACID	1	50
638675	N-TRICOSANE	6	01,05,06, 14,16,40
638686	TRIACONTANE	1	16
643583	2-METHYLBIPHENYL	2	09,39
694804	1-BROMO-2-CHLOROBENZENE	1	39

Confirmed Compounds
Sorted by CASRN

CASRN	Compound Name	# of occurrences of compound	IC's
697825	2,3,5-TRIMETHYLPHENOL	2	17,50
700129	PENTAMETHYLBENZENE	2	33,42
706149	GAMMA-DECALACTONE	1	12
719222	2,6-DI-TERT-BUTYL-P-BENZOQUINONE	1	21
767599	1-METHYL-1H-INDENE	2	12,12
791286	TRIPHENYLPHOSPHINE OXIDE	1	33
815247	2,2,4,4-TETRAMETHYL-3-PENTANONE	1	39
821556	METHYL HEPTYL KETONE	1	18
822866	TRANS,1,2-DICHLOROCYCLOHEXANE	2	33,33
829265	2,3,6-TRIMETHYLNAPHTHALENE	12	01,04,05, 06,08,11, 13,19,33, 40,42,50
832699	1-METHYLPHENANTHRENE	6	01,05,06, 11,33,40
872504	N-METHYL-2-PYRROLIDONE	1	21
874351	5-METHYL-(2,3-DIHYDROINDENE)(5-METHYLINDAN)	2	05,33
874419	1,3-DIMETHYL-4-ETHYLBENZENE	6	05,10,17, 19,27,40

Confirmed Compounds
Sorted by CASRN

CASRN	Compound Name	# of occurrences of compound	IC's
877430	2,6-DIMETHYLQUINOLINE	1	33
882337	DIPHENYL DISULFIDE	1	17
883205	9-METHYLPHENANTHRENE	5	01,04,05, 11,33
933755	2,3,6-TRICHLOROPHENOL	1	33
933982	3-ETHYL-O-XYLENE	4	05,19,33, 40
934747	5-ETHYL-M-XYLENE	12	04,05,06, 10,11,12, 19,20,27, 33,40,42
934805	1,2-DIMETHYL-4-ETHYLBENZENE	2	33,40
939275	2-ETHYLNAPHTHALENE	12	01,04,05, 08,11,12, 20,33,39, 40,42,50
1072839	2-ACETYLPYRROLE	1	99
1074175	1-METHYL-2-N-PROPYLBENZENE	8	05,10,14, 19,33,40, 42,50
1074437	1-METHYL-3-N-PROPYLBENZENE	2	08,33
1120214	N-UNDECANE	7	04,05,08, 09,19,20, 42

Confirmed Compounds
Sorted by CASRN

CASRN	Compound Name	# of occurrences of compound	IC's
1127760	1-ETHYLNAPHTHALENE	5	01,05,20, 39,40
1195795	FENCHONE	2	16,17
1490046	MENTHOL	1	12
1556996	4-METHYLFLUORENE	1	06
1570656	4,6-DICHLORO-O-CRESOL	1	12
1576676	3,6-DIMETHYLPHENANTHRENE	4	04,05,11, 33
1576698	2,7-DIMETHYLPHENANTHRENE	3	05,11,33
1632731	FENCHYL ALCOHOL	5	01,08,16, 17,33
1667012	2,4,6-TRIMETHYLACETOPHENONE	1	12
1678917	ETHYL-CYCLOHEXANE	1	40
1685821	4,6-DIMETHYLINDAN	3	01,05,50
1730376	1-METHYLFLUORENE	5	04,05,06, 33,40
1912249	ATRAZINE	1	98
1921706	2,6,10,14-TETRAMETHYL PENTADECANE	2	01,06

Confirmed Compounds
Sorted by CASRN

CASRN	Compound Name	# of occurrences of compound	IC's
2027170	2-ISOPROPYLNAPHTHALENE	5	05,06,08, 12,39
2033898	3,4-DIMETHOXYPHENOL	1	99
2078548	2,6-DIISOPROPYL PHENOL	1	16
2245387	2,3,5-TRIMETHYLNAPHTHALENE	9	05,06,08, 09,11,19, 33,36,39
2437561	1-TRIDECENE	1	10
2478388	ACETOSYRINGONE	1	16
2531842	2-METHYLPHENANTHRENE	3	01,04,40
2758181	3-METHYLCYCLOPENT-2-ENE-1-ONE	2	16,16
2847725	4-METHYLDECANE	2	05,40
2896608	4-ETHYLRESORCINOL	1	16
3209221	2,3-DICHLORONITROBENZENE	1	39
3442782	2-METHYLPYRENE	2	01,11
3622842	N-BUTYLBENZENESULPHONAMIDE	1	33
4170303	2-BUTENAL (CROTONALDEHYDE)	1	21
4706905	1-ISOPROPYL-3,5-DIMETHYLBENZENE	7	05,06,17, 19,33,40, 42

Confirmed Compounds
Sorted by CASRN

CASRN	Compound Name	# of occurrences of compound	IC's
6628188	1,2-BIS(METHYLMERCAPTO)ETHANE	1	16
6682719	4,7-DIMETHYLINDAN	5	01,05,06, 19,42
6975980	2-METHYLDECANE	1	05
7683649	SQUALENE	1	44
12002254	DIPROPYLENEGLYCOL METHYL ETHER	1	19
13466789	3-CARENE	3	16,16,17
14667551	TRIMETHYL PYRAZINE	1	40
18172673	BETA PINENE	2	16,16
20324338	TRIPROPYLENE GLYCOL METHYL ETHER	1	01
22239549	PARA-ALPHA-CUMYLPHENOL	1	39
25013165	BUTYLATED HYDROXY ANISOLE	1	12
29538770	TRANS-4-CHLOROCYCLOHEXANOL	1	33
35076927	1,4-DIBROMOCYCLOHEXANE	2	33,39
36563470	AR-BROMOPHENYL PHENYL ETHER	1	39
36653824	N-HEXADECANOL	3	14,39,50

Appendix E

Concentrations of Confirmed Compounds
Sorted by Industrial Code and CASRN

CASRN	Compound Name	RTI CONC ng/ul (extract)
AMUSEMENTS&ATHLETIC GOODS		
58902	2,3,4,6-TETRACHLOROPHENOL	69084
90120	1-METHYLNAPHTHALENE	83
91203	NAPHTHALENE	485
91576	2-METHYLNAPHTHALENE	199
95476	1,2-DIMETHYLBENZENE(O-XYLENE)	2806
98555	ALPHA-TERPINEOL	23
100414	ETHYLBENZENE	4985
104767	2-ETHYL-1-HEXANOL	26
106423	P-XYLENE	12285
107926	N-BUTYRIC ACID	446
108383	M-XYLENE	8190
111762	2-BUTOXYETHANOL	86740
111900	2-(2-ETHOXYETHOXY) ETHANOL	175
112345	2-(2-BUTOXYETHOXY)ETHANOL	5084
112390	METHYL HEXADECANOATE	5082
112403	N-DODECANE	395
124107	METHYL TETRADECANOATE	200
143077	LAURIC ACID	1096
488233	1,2,3,4-TETRAMETHYLBENZENE (PREHNITENE)	92
535773	1-METHYL-3-ISOPROPYLBENZENE	< .01
544638	MYRISTIC ACID	470
544763	HEXADECANE (PRACTICAL)	741
571584	1,4-DIMETHYLNAPHTHALENE	33
571619	1,5-DIMETHYLNAPHTHALENE	54
575417	1,3-DIMETHYLNAPHTHALENE	134
582161	2,7-DIMETHYLNAPHTHALENE	99
611143	O-ETHYLTOLUENE	75
629505	N-TRIDECANE	478
629594	N-TETRADECANE	563
700129	PENTAMETHYLBENZENE	44
829265	2,3,6-TRIMETHYLNAPHTHALENE	38
934747	5-ETHYL-M-XYLENE	90
939275	2-ETHYLNAPHTHALENE	120
1074175	1-METHYL-2-N-PROPYLBENZENE	13
1120214	N-UNDECANE	328
4706905	1-ISOPROPYL-3,5-DIMETHYLBENZENE	7
6682719	4,7-DIMETHYLINDAN	36
AUTO & OTHER LAUNDRIES		
51445	3,4-DICHLOROBENZOIC ACID	535
51445	3,4-DICHLOROBENZOIC ACID	872
54115	NICOTINE	29
58082	CAFFEINE	60

Concentrations of Confirmed Compounds
Sorted by Industrial Code and CASRN

AUTO & OTHER LAUNDRIES (Continued)

CASRN	Compound Name	RTI CONC ng/ul (extract)
79016	TRICHLOROETHYLENE	1534
79312	2-METHYLPROPANOIC ACID (ISOBUTYRIC ACID)	141
84742	DIBUTYL PHTHALATE	18
86748	CARBAZOLE	< 1
90120	1-METHYL NAPHTHALENE	21
91203	NAPHTHALENE	21
91576	2-METHYLNAPHTHALENE	220
95476	1,2-DIMETHYLBENZENE(O-XYLENE)	124
95636	1,2,4-TRIMETHYLBENZENE	52
95932	1,2,4,5-TETRAMETHYLBENZENE	133
98555	ALPHA-TERPINEOL	8
99876	P-CYMENE	104
100414	ETHYLBENZENE	135
100425	STYRENE	16
100425	STYRENE	14
103333	AZOBENZENE	123
103491	DIBENZYLAMINE	13
103651	N-PROPYLBENZENE	89
106445	PARA-CRESOL (4-METHYLPHENOL)	< 1
107926	BUTANOIC ACID (BUTYRIC ACID)	461
108383	M-XYLENE	175
108394	M-CRESOL	10
108678	1,3,5-TRIMETHYLBENZENE	155
108883	TOLUENE	457
108952	PHENOL	107
111148	HEPTANOIC ACID	21
111762	2-N-BUTOXYETHANOL	58
112050	NONANOIC ACID	34
112345	2-(2-BUTOXYETHOXY) ETHANOL	53
112345	2-(2-BUTOXYETHOXY) ETHANOL	244
112403	N-DODECANE	7
112618	METHYL STEARATE	16
112958	N-EICOSANE	965
120127	ANTHRACENE	1
124072	OCTANOIC ACID	139
124185	N-DECANE	39
135988	SEC-BUTYLBENZENE	3
141935	M-DIETHYLBENZENE	149
142621	HEXANOIC ACID(CAPROIC ACID)	249
143077	LAURIC ACID	61
334485	DECANOIC ACID	39
488233	1,2,3,4-TETRAMETHYLBENZENE (PREHNITENE)	24
496117	INDANE	160
526738	1,2,3-TRIMETHYLBENZENE	1832

Concentrations of Confirmed Compounds
Sorted by Industrial Code and CASRN

CASRN	Compound Name	RTI CONC ng/ul (extract)
AUTO & OTHER LAUNDRIES (Continued)		
527537	1,2,3,5-TETRAMETHYLBENZENE	110
527844	O-CYMENE	124
535773	1-METHYL-3-ISOPROPYLBENZENE	55
544763	HEXADECANE (PRACTICAL)	1011
571584	1,4-DIMETHYLNAPHTHALENE	7
571619	1,5-DIMETHYLNAPHTHALENE	35
575417	1,3-DIMETHYLNAPHTHALENE	22
575439	1,6-DIMETHYLNAPHTHALENE	7
593453	OCTADECANE	807
611143	1-METHYL-2-ETHYLBENZENE	285
620144	1-METHYL-3-ETHYLBENZENE	14
629505	N-TRIDECANE	59
629594	TETRADECANE	123
629629	N-PENTADECANE	683
629787	N-HEPTADECANE	319
629925	NONADECANE	573
629992	N-PENTACOSANE	1
630013	N-HEXACOSANE	2
829265	2,3,6-TRIMETHYLNAPHTHALENE	8
874419	1,3-DIMETHYL-4-ETHYLBENZENE	2132
933982	3-ETHYL-O-XYLENE	67
934747	5-ETHYL-M-XYLENE	193
1074175	1-METHYL-2-N-PROPYLBENZENE	188
1120214	N-UNDECANE	2019
2245387	2,3,5-TRIMETHYLNAPHTHALENE	6
4706905	1-ISOPROPYL-3,5-DIMETHYLBENZENE	4
6682719	4-7 DIMETHYLINDAN	5
12002254	DIPROPYLENEGLYCOL METHYL ETHER	476
COAL MINING		
85018	PHENANTHRENE	5
86737	FLUORENE	3
90120	1-METHYL NAPHTHALENE	72
91203	NAPHTHALENE	41
91576	2-METHYLNAPHTHALENE	194
95487	O-CRESOL	4
99876	P-CYMENE	5
106423	1,4-DIMETHYLBENZENE(P-XYLENE)	155
108101	4-METHYL-2-PENTANONE	138
108383	M-XYLENE	225
108689	3,5-XYLENOL	2
112345	2-(2-BUTOXYETHOXY)ETHANOL	7
112403	NOR-DODECANE	37

Concentrations of Confirmed Compounds
Sorted by Industrial Code and CASRN

CASRN	Compound Name	RTI CONC ng/ul (extract)
COAL MINING	(Continued)	
112958	N-EICOSANE	
117817	DI-(2-ETHYLHEXYL)PHTHALATE	60
120127	ANTHRACENE	6
127184	TETRACHLOROETHYLENE	18
128370	(2,6-DI-TERT-BUTYL-4-METHYL PHENOL)	703
132649	DIBENZOFURAN (DIPHENYLENE OXIDE)	< 1
135988	SEC-BUTYLBENZENE	14
243174	2,3 BENZOFLUORENE	3
527844	O-CYMENE	13
544763	HEXADECANE	5
571619	1,5-DIMETHYLNAPHTHALENE	26
575417	1,3-DIMETHYLNAPHTHALENE	9
575439	1,6-DIMETHYLNAPHTHALENE	0
576261	2,6-DIMETHYL PHENOL	40
581420	2,6-DIMETHYLNAPHTHALENE	< .01
582161	2,7-DIMETHYLNAPHTHALENE	19
593453	OCTADECANE	32
611143	1-METHYL-2-ETHYLBENZENE	6
613127	2-METHYL ANTHRACENE	< 1
616239	2,3-DICHLORO-1-PROPANOL	< 1
620144	M-ETHYLTOLUENE	5
622968	1-METHYL-4-ETHYLBENZENE	3
629505	N-TRIDECANE	14
629594	TETRADECANE	30
629629	PENTADECANE	30
629925	NONADECANE	40
829265	2,3,6-TRIMETHYLNAPHTHALENE	6
832699	1-METHYLPHENANTHRENE	16
883205	9-METHYLPHENANTHRENE	5
934747	5-ETHYL-M-XYLENE	2
939275	2-ETHYLNAPHTHALENE	3
1576676	3,6-DIMETHYLPHENANTHRENE	31
1576698	2,7-DIMETHYLPHENANTHRENE	27
2245387	2,3,5-TRIMETHYLNAPHTHALENE	0
3442782	2-METHYLPYRENE	14
		16
ELECTRONICS		
58902	2,3,4,6-TETRACHLOROPHENOL	
65850	BENZOIC ACID	840
67710	DIMETHYL SULFONE	87020
71432	BENZENE	10
83330	INDAN-1-ONE	743
84742	BUTYL PHTHALATE	73
		1

Concentrations of Confirmed Compounds
Sorted by Industrial Code and CASRN

ELECTRONICS (Continued)

CASRN	Compound Name	RTI CONC ng/ul (extract)
85018	PHENANTHRENE	43
87616	1,2,3-TRICHLOROBENZENE	922
87650	2,6-DICHLOROPHENOL	2
88755	ORTHO-NITROPHENOL	13
90006	O-ETHYLPHENOL	41
90120	1-METHYLNAPHTHALENE	460
90437	O-PHENYLPHENOL	265
91203	NAPHTHALENE	136
91576	2-METHYLNAPHTHALENE	1181
95169	BENZOTHIAZOLE	108
95169	BENZOTHIAZOLE	36
95476	1,2-DIMETHYLBENZENE(O-XYLENE)	89
95501	ORTHO-DICHLOROBENZENE	2303
95636	1,2,4-TRIMETHYLBENZENE	28
95932	1,2,4,5-TETRAMETHYLBENZENE	42
95954	2,4,5-TRICHLOROPHENOL	374
98011	FURFURAL	7775
98544	P-TERT BUTYLPHENOL	128
98555	ALPHA-TERPINEOL	2048
98555	ALPHA-TERPINEOL	< 1
98737	P-TERT-BUTYLBENZOIC ACID	280449
98862	METHYL-PHENYL KETONE	42
99047	M-TOLUIC ACID	860
99876	P-CYMENE	< 1
100414	ETHYLBENZENE	268
101848	PHENYL ETHER	35
103822	PHENYLACETIC ACID	152
104767	2-ETHYL-1-HEXANOL	57
106423	1,4-DIMETHYLBENZENE(P-XYLENE)	0
106445	PARA-CRESOL (4-METHYLPHENOL)	5
106467	P-DICHLOROBENZENE	292
107142	CHLOROETHANENITRILE(CHLOROACETONITRILE)	315
108101	4 METHYL-PENTANONE 2	306
108383	M-XYLENE	54
108678	1,3,5-TRIMETHYLBENZENE	7
108883	TOLUENE	167
108952	PHENOL	129
109524	PENTANOIC ACID (VALERIC ACID)	286
110430	HEPTAN-2-ONE	1481
110805	2-ETHOXYETHANOL (ETHYLENE GLYCOL MONOETHYL ETHER)	446
110838	CYCLOHEXENE	83
111762	2-N-BUTOXYETHANOL	83
112050	NONANOIC ACID	364
112050	NONANOIC ACID	2720

Concentrations of Confirmed Compounds
Sorted by Industrial Code and CASRN

ELECTRONICS (Continued)

CASRN -----	Compound Name -------------	RTI CONC -------- ng/ul (extract)
112254	2-HEXYLOXYETHANOL	18300
112345	2-(2-BUTOXYETHOXY)ETHANOL	214
112403	NOR-DODECANE	854
112958	N-EICOSANE	9928
115195	2-METHYL-3-BUTYN-2-OL	7646
118901	O-TOLUIC ACID	863
120127	ANTHRACENE	871
120821	1,2,4-TRICHLOROBENZENE	82
121335	VANILLIN (4-HYDROXY-3-METHOXY BENZALDEHYDE)	40
124072	OCTANOIC ACID	114
124185	N-DECANE	118
135988	SEC-BUTYLBENZENE	48
142621	HEXANOIC ACID(CAPROIC ACID)	8604
334485	DECANOIC ACID	2156
367124	O-FLUOROPHENOL	11
488233	1,2,3,4-TETRAMETHYLBENZENE (PREHNITENE)	27
488233	1,2,3,4-TETRAMETHYLBENZENE (PREHNITENE)	< 1
507700	1-BORNEOL	255
527537	1,2,3,5-TETRAMETHYLBENZENE	220
527844	1-METHYL-2-ISOPROPYLBENZENE	42
540385	P-IODOPHENOL	217
541731	M-DICHLOROBENZENE	26
544638	MYRISTIC ACID	5513
544763	HEXADECANE (PRACTICAL)	1172
544763	HEXADECANE (PRACTICAL)	326
571584	1,4-DIMETHYLNAPHTHALENE	84
571619	1,5-DIMETHYLNAPHTHALENE	86
575417	1,3-DIMETHYLNAPHTHALENE	8
575439	1,6-DIMETHYLNAPHTHALENE	458
582161	2,7-DIMETHYLNAPHTHALENE	223
585342	M-TERT-BUTYLPHENOL	68
593453	OCTADECANE	1358
610720	2,5-DIMETHYL-BENZOIC ACID	524
611018	2,4-DIMETHYL-BENZOIC ACID	3063
611143	O-ETHYLTOLUENE	8
619045	3,4-DIMETHYL-BENZOIC ACID	1904
620144	M-ETHYLTOLUENE	48
622968	1-METHYL-4-ETHYLBENZENE	9
629505	TRIDECANE	2643
629594	TETRADECANE	141
629629	N-PENTADECANE	2947
629787	HEPTADECANE	558
629925	NONADECANE	847
629992	N-PENTACOSANE	12

Concentrations of Confirmed Compounds
Sorted by Industrial Code and CASRN

CASRN	Compound Name	RTI CONC ng/ul (extract)
ELECTRONICS	(Continued)	
630013	N-HEXACOSANE	3190
630206	1,1,1,2-TETRACHLOROETHANE	163
700129	PENTAMETHYLBENZENE	56
791286	TRIPHENYLPHOSPHINE OXIDE	4
822866	TRANS,1,2-DICHLOROCYCLOHEXANE	485
822866	TRANS,1,2-DICHLOROCYCLOHEXANE	142
829265	2,3,6-TRIMETHYLNAPHTHALENE	2281
832699	1-METHYLPHENANTHRENE	61
874351	5-METHYL-(2,3-DIHYDROINDENE)(5-METHYLINDAN)	13
877430	2,6-DIMETHYLQUINOLINE	< .01
883205	9-METHYLPHENANTHRENE	31
933755	2,3,6-TRICHLOROPHENOL	31
933982	3-ETHYL-O-XYLENE	11
934747	5-ETHYL-M-XYLENE	20
934805	1,2-DIMETHYL-4-ETHYLBENZENE	26
939275	2-ETHYLNAPHTHALENE	5
1074175	1-METHYL-2-N-PROPYLBENZENE	14
1074437	1-METHYL-3-N-PROPYLBENZENE	3
1576676	3,6-DIMETHYLPHENANTHRENE	19
1576698	2,7-DIMETHYLPHENANTHRENE	44
1632731	FENCHYL ALCOHOL	118
1730376	1-METHYLFLUORENE	5
2245387	2,3,5-TRIMETHYLNAPHTHALENE	114
3622842	N-BUTYLBENZENESULPHONAMIDE	10
4706905	1-ISOPROPYL-3,5-DIMETHYLBENZENE	18
29538770	TRANS-4-CHLOROCYCLOHEXANOL	9
35076927	1,4-DIBROMOCYCLOHEXANE	321
EXPLOSIVES		
91203	NAPHTHALENE	< 1
98011	FURFURAL	124
120127	ANTHRACENE	< 1
FOUNDRIES		
85687	BUTYL BENZYL PHTHALATE	1
91203	NAPHTHALENE	< 1
108952	PHENOL	< 1
112345	2-(2-BUTOXYETHOXY)ETHANOL	3
117817	DI-(2-ETHYLHEXYL)PHTHALATE	19
INDUSTRY UNKNOWN		
57103	PALMITIC ACID	134

Concentrations of Confirmed Compounds
Sorted by Industrial Code and CASRN

CASRN	Compound Name	RTI CONC ng/ul (extract)
INDUSTRY UNKNOWN	(Continued)	
58082	CAFFEINE	14
92524	BIPHENYL	47
95498	O-CHLOROTOLUENE	6
98555	ALPHA-TERPINEOL	4
100516	BENZYL ALCOHOL	729
101848	DIPHENYLETHER	124
112345	2-(2-BUTOXYETHOXY)ETHANOL	141
112345	2-(2-BUTOXYETHOXY) ETHANOL	26
117817	DI-(2-ETHYLHEXYL)PHTHALATE	5
127184	TETRACHLOROETHYLENE	1226
1912249	ATRAZINE	3805
INORGANIC CHEMICALS		
71363	1-BUTANOL	60
84662	DIETHYL PHTHALATE	9
88722	ORTHO-NITROTOLUENE	161
90437	1-HYDROXY-2-PHENYLBENZENE	63
91203	NAPHTHALENE	116
91576	2-METHYLNAPHTHALENE	20
95476	1,2-DIMETHYLBENZENE(O-XYLENE)	198
95487	O-CRESOL	7
95501	Benzene,1,2-dichloro-	2101
95534	O-TOLUIDINE	586
95578	O-CHLOROPHENOL	7
95636	1,2,4-TRIMETHYLBENZENE	7
95954	2,4,5-TRICHLOROPHENOL	51
98555	ALPHA-TERPINEOL	4
98828	ISOPROPYLBENZENE	10
98953	Benzene,nitro-	240151
99990	PARA-NITROTOLUENE	922
100414	ETHYLBENZENE	141
100425	STYRENE	17
106423	1,4-DIMETHYLBENZENE(P-XYLENE)	604
106467	P-DICHLOROBENZENE	< 1
108383	M-XYLENE	50
108678	1,3,5-TRIMETHYLBENZENE	2
108883	TOLUENE	398
108883	TOLUENE	26
110861	PYRIDINE	211
112345	2-(2-BUTOXYETHOXY)ETHANOL	36
112958	N-EICOSANE	2
121142	2,4-DINITROTOLUENE	12207
121335	VANILLIN	2

Concentrations of Confirmed Compounds
Sorted by Industrial Code and CASRN

INORGANIC CHEMICALS (Continued)

CASRN	Compound Name	RTI CONC ng/ul (extract)
122394	DIPHENYLAMINE	11
128370	(2,6-DI-TERT-BUTYL-4-METHYL PHENOL)	29
135988	SEC-BUTYLBENZENE	4
486259	FLUORENONE	< 1
498022	4-HYDROXY-3-METHOXYACETOPHENONE	< 1
507700	BORNEOL	1
526738	1,2,3-TRIMETHYLBENZENE	7
529340	ALPHA-TETRALONE	9
582161	2,7-DIMETHYLNAPHTHALENE	< 1
606202	2,6-DINITROTOLUENE	2025
611143	O-ETHYLTOLUENE	72
611143	O-ETHYLTOLUENE	1
611154	O-METHYLSTYRENE	< 1
620144	M-ETHYLTOLUENE	8
622968	1-METHYL-4-ETHYLBENZENE	39
629594	N-TETRADECANE	2
829265	2,3,6-TRIMETHYLNAPHTHALENE	< 1

IRON & STEEL MFG.

CASRN	Compound Name	RTI CONC ng/ul (extract)
56553	1,2-BENZANTHRACENE	4
85018	PHENANTHRENE	279
88697	ORTHO-ISOPROPYLPHENOL (ORTHO-CUMENOL)	18
90120	1-METHYL NAPHTHALENE	216
90437	O-PHENYLPHENOL	129
91203	NAPHTHALENE	25
91225	QUINOLINE (1-BENZAZINE)	663
91576	2-METHYLNAPTHALENE	637
91576	2-METHYLNAPHTHALENE	430
95487	O-CRESOL	446
95636	1,2,4-TRIMETHYLBENZENE	68
99876	P-CYMENE	9
103822	PHENYLACETIC ACID	114
105679	2,4-XYLENOL	472
107415	2-METHYL-2,4-PENTANEDIOL	473
108394	M-CRESOL	873
108952	PHENOL	21089
111900	DIETHYLENE GLYCOL MONOETHYL ETHER	497
112390	METHYL PALMITATE	284
112403	DODECANE	2235
120127	ANTHRACENE	190
120729	INDOLE	150
123079	PARA-ETHYLPHENOL	6
129000	PYRENE	494

Concentrations of Confirmed Compounds
Sorted by Industrial Code and CASRN

IRON & STEEL MFG. (Continued)

CASRN	Compound Name	RTI CONC ng/ul (extract)
132649	DIBENZOFURAN	50
206440	FLUORANTHENE	393
207089	BENZO(K)FLUORANTHENE	96
208968	ACENAPHTHALENE	22
218019	CHRYSENE	61
526738	1,2,3-TRIMETHYLBENZENE	8
535773	1-METHYL-3-ISOPROPYLBENZENE	101
544763	N-HEXADECANE	2175
571619	1,5-DIMETHYLNAPHTHALENE	165
575417	1,3-DIMETHYLNAPHTHALENE	183
575439	1,6-DIMETHYLNAPHTHALENE	0
582161	2,7-DIMETHYLNAPHTHALENE	256
593453	N-OCTADECANE	1179
611143	O-ETHYLTOLUENE	34
622968	1-METHYL-4-ETHYLBENZENE	138
629505	N-TRIDECANE	10
629594	N-TETRADECANE	8
629787	N-HEPTADECANE	1306
629925	NONADECANE	22
829265	2,3,6-TRIMETHYLNAPHTHALENE	943
883205	9-METHYLPHENANTHRENE	139
934747	5-ETHYL-M-XYLENE	83
939275	2-ETHYLNAPHTHALENE	120
1120214	N-UNDECANE	1165
1576676	3,6-DIMETHYLPHENANTHRENE	48
1730376	1-METHYLFLUORENE	26
2531842	2-METHYLPHENANTHRENE	25

LEATHER TANNING

CASRN	Compound Name	RTI CONC ng/ul (extract)
90051	O-METHOXYPHENOL (GUAIACOL)	6
90120	1-METHYLNAPHTHALENE	13
91203	NAPHTHALENE	3
91576	2-METHYLNAPHTHALENE	14
94597	SAFROLE	7
95501	O-DICHLOROBENZENE	16
95954	2,4,5-TRICHLOROPHENOL	18
98555	ALPHA-TERPINEOL	78
106445	PARA-CRESOL (4-METHYLPHENOL)	29
107926	N-BUTYRIC ACID	267
108394	META-CRESOL (3-METHYLPHENOL)	0
108883	TOLUENE	13
108952	PHENOL	2057
109524	VALERIC ACID	3418

Concentrations of Confirmed Compounds
Sorted by Industrial Code and CASRN

CASRN	Compound Name	RTI CONC ng/ul (extract)
LEATHER TANNING	(Continued)	
120729	INDOLE	11
121335	VANILLIN (4-HYDROXY-3-METHOXY BENZALDEHYDE)	5
127184	TETRACHLOROETHYLENE	798
138863	LIMONENE	160
291214	1,3,5-TRITHIANE	63
541731	M-DICHLOROBENZENE	10
582161	2,7-DIMETHYLNAPHTHALENE	15
MECHANICAL PRODUCTS		
54115	NICOTINE	70
56553	1,2-BENZANTHRACENE	< 1
57103	PALMITIC ACID	7386
58082	CAFFEINE	114
58902	2,3,4,6-TETRACHLOROPHENOL	142479
59507	4-CHLORO-M-CRESOL	1587
65850	BENZOIC ACID	680852
76222	NORBORNAN-2-ONE (CAMPHOR)	3
90120	1-METHYLNAPHTHALENE	115
90437	O-PHENYLPHENOL	382
91203	NAPHTHALENE	89
91576	2-METHYLNAPTHALENE	295
94597	SAFROLE	49
95169	BENZOTHIAZOLE	48
95169	BENZOTHIAZOLE	65
95476	1,2-DIMETHYLBENZENE(O-XYLENE)	34
95636	1,2,4-TRIMETHYLBENZENE	157
98544	P-TERT BUTYLPHENOL	56
98555	ALPHA-TERPINEOL	80
98555	ALPHA-TERPINEOL	453
98555	ALPHA-TERPINEOL	56
98828	ISOPROPYLBENZENE	82
98851	1-PHENYLETHANOL	63
98862	METHYL-PHENYL KETONE	32
99047	M-TOLUIC ACID	77
99876	P-CYMENE	< 1
100414	ETHYLBENZENE	1259
103822	PHENYLACETIC ACID	4396
106423	1,4-DIMETHYLBENZENE(P-XYLENE)	5395
106445	PARA-CRESOL (4-METHYLPHENOL)	< 1
107415	2-METHYL-2,4-PENTANEDIOL	145
108383	1,3-DIMETHYLBENZENE(M-XYLENE)	15
108883	TOLUENE	< .01
108952	PHENOL	52

Concentrations of Confirmed Compounds
Sorted by Industrial Code and CASRN

MECHANICAL PRODUCTS (Continued)

CASRN	Compound Name	RTI CONC ng/ul (extract)
109524	PENTANOIC ACID (VALERIC ACID)	33
111148	HEPTANOIC ACID	1393
112050	NONANOIC ACID	1954
112618	STEARIC ACID METHYL ESTER	1788
112958	N-EICOSANE	1177
115866	TRI-PHENYL PHOSPHATE	27
119619	BENZOPHENONE	6
122996	2-PHENOXYETHANOL	8
123079	PARA-ETHYLPHENOL	< 1
124072	CAPRYLIC ACID	4976
124185	N-DECANE	9807
129000	PYRENE	8
135013	1,2-DIETHYLBENZENE	13
142621	HEXANOIC ACID(CAPROIC ACID)	6388
507700	BORNEOL	4
526738	1,2,3-TRIMETHYLBENZENE	782
544763	N-HEXADECANE	154
569415	1,8-DIMETHYLNAPHTHALENE	93
571584	1,4-DIMETHYLNAPHTHALENE	< 1
571619	1,5-DIMETHYLNAPHTHALENE	80
575417	1,3-DIMETHYLNAPHTHALENE	63
575439	1,6-DIMETHYLNAPHTHALENE	89
581408	2,3-DIMETHYLNAPHTHALENE	16
582161	2,7-DIMETHYLNAPHTHALENE	88
593453	OCTADECANE	122
605027	Naphthalene,1-phenyl-	1
611143	O-ETHYLTOLUENE	128
620144	1-METHYL-3-ETHYLBENZENE	34
629505	N-TRIDECANE	21
629594	TETRADECANE	207
629629	PENTADECANE	162
629787	HEPTADECANE	245
629925	NONADECANE	464
629992	N-PENTACOSANE	16
638675	N-TRICOSANE	256
829265	2,3,6-TRIMETHYLNAPHTHALENE	48
832699	1-METHYLPHENANTHRENE	7
874419	1,3-DIMETHYL-4-ETHYLBENZENE	820
933982	3-ETHYL-O-XYLENE	12
934747	1,3-DIMETHYL-5-ETHYLBENZENE	62
934805	1,2-DIMETHYL-4-ETHYLBENZENE	2199
939275	2-ETHYLNAPHTHALENE	85
1074175	1-METHYL-2-N-PROPYLBENZENE	404
1127760	1-ETHYLNAPHTHALENE	83

Concentrations of Confirmed Compounds
Sorted by Industrial Code and CASRN

CASRN	Compound Name	RTI CONC ng/ul (extract)
MECHANICAL PRODUCTS	(Continued)	
1678917	ETHYL-CYCLOHEXANE	82
1730376	1-METHYLFLUORENE	219
2531842	2-METHYLPHENANTHRENE	9
2847725	4-METHYLDECANE	1500
4706905	1-ISOPROPYL-3,5-DIMETHYLBENZENE	5
14667551	TRIMETHYL PYRAZINE	965
NONFERROUS METALS		
65850	BENZOIC ACID	3694
70553	P-TOLUENESULPHONAMIDE	22
71432	BENZENE	10
75741	TETRAMETHYLLEAD	554
84742	DIBUTYL PHTHALATE	65
84764	DINONYL PHTHALATE	406
85018	PHENANTHRENE	1
85687	BUTYL BENZYL PHTHALATE	2152
90120	1-METHYLNAPHTHALENE	0
90302	1-Naphthalenamine,N-phenyl-	< 1
91203	NAPHTHALENE	18
91576	2-METHYLNAPHTHALENE	116
99876	1-METHYL-4-ISOPROPYLBENZENE	10
100516	BENZYL ALCOHOL	100
100527	BENZALDEHYDE	5
104405	P-NONYLPHENOL	3
104767	2-ETHYL-1-HEXANOL	7
106423	P-XYLENE	10
107415	2-METHYL-2,4-PENTANEDIOL	14
108383	M-XYLENE	2
108952	PHENOL	830
112390	METHYL N-HEXADECANOATE	496
112403	NOR-DODECANE	97
112538	DODECANOL	18
112618	STEARIC ACID METHYL ESTER	94
112629	METHYL OLEATE	6580
112958	N-EICOSANE	14
115866	TRI-PHENYL PHOSPHATE	9
117840	DIOCTYL PHTHALATE	22083
120127	ANTHRACENE	16
121335	VANILLIN	710
127184	TETRACHLOROETHYLENE	120
129000	PYRENE	1514
132650	DIBENZOTHIOPHENE	< 1
150787	P-DIMETHOXYBENZENE	< 1

Concentrations of Confirmed Compounds
Sorted by Industrial Code and CASRN

CASRN	Compound Name	RTI CONC ng/ul (extract)
NONFERROUS METALS	(Continued)	
206440	FLUORANTHENE	13
501520	PHENYLPROPIONIC ACID	271
535773	M-CYMENE	6
544763	N-HEXADECANE	111
571584	1,4-DIMETHYLNAPHTHALENE	0
571619	1,5-DIMETHYLNAPHTHALENE	54
575417	1,3-DIMETHYLNAPHTHALENE	51
593453	OCTADECANE	12
613127	2-METHYL ANTHRACENE	31
629505	N-TRIDECANE	227
629594	N-TETRADECANE	99
629629	PENTADECANE	1171
629787	HEPTADECANE	129
629925	NONADECANE	84
638675	N-TRICOSANE	3
829265	2,3,6-TRIMETHYLNAPHTHALENE	62
832699	1-METHYLPHENANTHRENE	82
934747	5-ETHYL-M-XYLENE	1
1556996	4-METHYLFLUORENE	74
1730376	1-METHYLFLUORENE	2
1921706	2,6,10,14-TETRAMETHYL PENTADECANE	64
2027170	2-ISOPROPYLNAPHTHALENE	14
2245387	2,3,5-TRIMETHYLNAPHTHALENE	164
4706905	1-ISOPROPYL-3,5-DIMETHYLBENZENE	11
6682719	4,7-DIMETHYLINDAN	18
OIL AND GAS EXTRACTION		
91203	NAPHTHALENE	1
91576	2-METHYLNAPHTHALENE	5
109524	PENTANOIC ACID (VALERIC ACID)	36
573988	Naphthalene,1,2-dimethyl-	< 1
575417	1,3-DIMETHYLNAPHTHALENE	0
575439	1,6-DIMETHYLNAPHTHALENE	4
582161	2,7-DIMETHYLNAPHTHALENE	3
2245387	2,3,5-TRIMETHYLNAPHTHALENE	< 1
ORE MINING		
65850	BENZOIC ACID	352
88062	2,4,6-TRICHLOROPHENOL	14
90120	1-METHYLNAPHTHALENE	35
91203	NAPHTHALENE	61
91576	2-METHYLNAPHTHALENE	65

Concentrations of Confirmed Compounds
Sorted by Industrial Code and CASRN

CASRN	Compound Name	RTI CONC ng/ul (extract)
ORE MINING	(Continued)	
95636	1,2,4-TRIMETHYLBENZENE	56
106423	1,4-DIMETHYLBENZENE(P-XYLENE)	8
108383	1,3-DIMETHYLBENZENE(M-XYLENE)	8
108678	1,3,5-TRIMETHYLBENZENE	19
111148	HEPTANOIC ACID	16
112050	NONANOIC ACID	12
112403	N-DODECANE	159
124072	OCTANOIC ACID	43
124185	N-DECANE	29
128370	(2,6-DI-TERT-BUTYL-4-METHYL PHENOL)	2
135988	SEC-BUTYLBENZENE	< 1
142621	HEXANOIC ACID(CAPROIC ACID)	3
334485	DECANOIC ACID	< 1
488233	1,2,3,4-TETRAMETHYLBENZENE (PREHNITENE)	12
526738	1,2,3-TRIMETHYLBENZENE	44
544763	HEXADECANE (PRACTICAL)	50
571619	1,5-DIMETHYLNAPHTHALENE	4
575417	1,3-DIMETHYLNAPHTHALENE	11
575439	1,6-DIMETHYLNAPHTHALENE	13
582161	2,7-DIMETHYLNAPHTHALENE	8
611143	1-METHYL-2-ETHYLBENZENE	16
620144	1-METHYL-3-ETHYLBENZENE	2
622968	P-ETHYLTOLUENE	16
629594	N-TETRADECANE	138
629629	N-PENTADECANE	65
874419	1,3-DIMETHYL-4-ETHYLBENZENE	187
934747	5-ETHYL-M-XYLENE	10
1074175	1-METHYL-2-N-PROPYLBENZENE	9
2437561	1-TRIDECENE	< 1
ORGANIC CHEMICALS		
64197	ETHANOIC ACID (ACETIC ACID)	6750
67721	HEXACHLOROETHANE	124
79312	ISOBUTYRIC ACID	11723
83329	ACENAPHTHENE	19
84742	BUTYL PHTHALATE	391
84742	BUTYL PHTHALATE	29
85018	PHENANTHRENE	47
86737	FLUORENE	9
87616	1,2,3-TRICHLOROBENZENE	4842
88062	2,4,6-TRICHLOROPHENOL	23
90120	1-METHYLNAPHTHALENE	348
91203	NAPHTHALENE	349

Concentrations of Confirmed Compounds
Sorted by Industrial Code and CASRN

ORGANIC CHEMICALS (Continued)

CASRN	Compound Name	RTI CONC ng/ul (extract)
91576	2-METHYLNAPHTHALENE	983
92524	DIPHENYL	88
93550	PROPIOPHENONE	29
93583	METHYL BENZOATE	265
95476	O-XYLENE	17
95487	O-CRESOL	248
95498	1-METHYL-2-CHLOROBENZENE (O-CHLOROTOLUENE)	1963
95501	O-DICHLOROBENZENE	47
95512	2-CHLOROANILINE	336
95578	O-CHLOROPHENOL	653
95636	1,2,4-TRIMETHYLBENZENE	61
95943	1,2,4,5-TETRACHLOROBENZENE	36
98544	P-TERT BUTYLPHENOL	1851
98862	PHENYL METHYL KETONE	1363
99036	M-AMINOACETOPHENONE	341
99627	1,3-DIISOPROPYLBENZENE	348
99752	P-TOLUIC ACID,METHYL ESTER	1101
100185	P-DIISOPROPYLBENZENE	100
100414	ETHYLBENZENE	31
100414	ETHYLBENZENE	2010
100470	BENZONITRILE (CYANOBENZENE)	176
100516	BENZYL ALCOHOL	157
100516	BENZYL ALCOHOL	69
101815	DIPHENYLMETHANE	270
101848	DIPHENYLETHER	1620
103811	2-PHENYLACETAMIDE	881
103822	PHENYLACETIC ACID	4568
104405	P-NONYLPHENOL	187
104767	2-ETHYL-1-HEXANOL	70
104905	2-METHYL-5-ETHYLPYRIDINE	3021
105679	2,4-XYLENOL	45
106423	1,4-DIMETHYLBENZENE(P-XYLENE)	229
106467	1,4-DICHLOROBENZENE	1623
108101	4-METHYL-2-PENTANONE	36
108372	1-BROMO-3-CHLOROBENZENE	2
108383	1,3-DIMETHYLBENZENE(M-XYLENE)	3579
108689	3,5-DIMETHYL PHENOL	9
108883	TOLUENE	424
108907	CHLOROBENZENE	6
108952	PHENOL	9998
111762	2-N-BUTOXYETHANOL	2940
112403	NOR-DODECANE	21
112425	1-UNDECANOL	17
112958	N-EICOSANE	197

Concentrations of Confirmed Compounds
Sorted by Industrial Code and CASRN

ORGANIC CHEMICALS (Continued)

CASRN	Compound Name	RTI CONC ng/ul (extract)
117840	DIOCTYL PHTHALATE	2075
118901	O-TOLUIC ACID	2613
119335	2-NITRO-P-CRESOL	66
120127	ANTHRACENE	6
120616	DIMETHYLTEREPHTHALATE	557
120821	1,2,4 TRICHLOROBENZENE	15757
120832	2,4-DICHLOROPHENOL	357
123911	P-DIOXANE	2425
128370	(2,6-DI-TERT-BUTYL-4-METHYL PHENOL)	34
139662	DIPHENYL SULFIDE	48
141797	4-METHYL-3-PENTEN-2-ONE	82
141935	M-DIETHYLBENZENE	24
143226	TRIETHYLENE GLYCOL N-BUTYL ETHER	160
259790	BIPHENYLENE	241
496117	2,3-DIHYDROINDENE	107
504201	2,6-DIMETHYL-2,5-HEPTADIEN-4-ONE	19
526738	1,2,3-TRIMETHYLBENZENE	5
529340	1-TETRALONE	42
535773	M-CYMENE	4
544763	N-HEXADECANE	11
554007	2,4-DICHLOROANILINE	22
571584	1,4-DIMETHYLNAPHTHALENE	33
575417	1,3-DIMETHYLNAPHTHALENE	80
575439	1,6-DIMETHYLNAPHTHALENE	63
593453	OCTADECANE	35
608275	2,3-DICHLOROANILINE	17
611143	O-ETHYLTOLUENE	169
611154	O-METHYLSTYRENE	4
614006	METHYLPHENYLNITROSOAMINE	9
619045	3,4-DIMETHYL-BENZOIC ACID	227
620144	1-METHYL-3-ETHYLBENZENE	0
620177	META-ETHYLPHENOL	125
622968	P-ETHYLTOLUENE	62
629505	N-TRIDECANE	64
629594	N-TETRADECANE	96
629629	N-PENTADECANE	8
643583	2-METHYLBIPHENYL	13
694804	1-BROMO-2-CHLOROBENZENE	9
815247	2,2,4,4-TETRAMETHYL-3-PENTANONE	17
939275	2-ETHYLNAPHTHALENE	442
1127760	1-ETHYLNAPHTHALENE	21
2027170	2-ISOPROPYLNAPHTHALENE	17
2245387	2,3,5-TRIMETHYLNAPHTHALENE	24
3209221	2,3-DICHLORONITROBENZENE	6936

Concentrations of Confirmed Compounds
Sorted by Industrial Code and CASRN

ORGANIC CHEMICALS (Continued)

CASRN	Compound Name	RII CONC ng/ul (extract)
22239549	PARA-ALPHA-CUMYLPHENOL	25
35076927	1,4-DIBROMOCYCLOHEXANE	65
36563470	AR-BROMOPHENYL PHENYL ETHER	2
36653824	1-HEXADECANOL	156

ORGANICS & PLASTICS

CASRN	Compound Name	RII CONC ng/ul (extract)
58902	2,3,4,6-TETRACHLOROPHENOL	2982
60093	4-AMINO-AZOBENZENE	929
60128	2-PHENYL ETHANOL	182
62533	ANILINE	2310
67663	CHLOROFORM	37
68122	N,N-DIMETHYLFORMAMIDE	13
69727	SALICYLIC ACID	28378
82053	BENZANTHRONE	5
84651	9,10-ANTHRAQUINONE	265
84662	DIETHYL PHTHALATE	351
84742	DIBUTYL PHTHALATE	17
85687	BUTYL BENZYL PHTHALATE	1758
86737	FLUORENE	42
87865	PENTACHLOROPHENOL	626
88062	2,4,6-TRICHLOROPHENOL	97
89634	4-CHLORO-2-NITROANILINE	246
90028	SALICYLALDEHYDE	1953
90051	ORTHO-METHOXYPHENOL	590
90120	1-METHYL NAPHTHALENE	30
90437	O-HYDROXYDIPHENYL	217
91203	NAPHTHALENE	225
92524	BIPHENYL	< 1
92524	BIPHENYL	26
92842	PHENOTHIAZINE	551
93583	METHYL BENZOATE	260
95487	O-CRESOL	283
95487	ORTHO-CRESOL (2-METHYLPHENOL)	36
95498	1-METHYL-2-CHLOROBENZENE (O-CHLOROTOLUENE)	305
95501	O-DICHLOROBENZENE	937
95761	3,4-DICHLOROANILINE	239
95954	2,4,5-TRICHLOROPHENOL	580
98544	P-TERT BUTYLPHENOL	< 1
98953	NITROBENZENE	17092
98953	NITROBENZENE	181
98953	NITROBENZENE	244
98953	NITROBENZENE	37
99309	2,6-DICHLORO-4-NITROANILINE	167

Concentrations of Confirmed Compounds
Sorted by Industrial Code and CASRN

CASRN -----	Compound Name -------------	RTI CONC -------- ng/ul (extract)
ORGANICS & PLASTICS	(Continued)	
99650	1,3-DINITROBENZENE	1055
100016	P-NITROANILINE	5680
100425	STYRENE	3
100425	STYRENE	6
100516	BENZYL ALCOHOL	1893
100527	BENZALDEHYDE	1
101815	DIPHENYLMETHANE	< 1
101848	DIPHENYLETHER	388
101848	DIPHENYLETHER	69
103822	PHENYLACETIC ACID	42766
103822	Benzeneaceticacid	3
104767	2-ETHYL-1-HEXANOL	74
104949	4-METHOXYANILINE	111
105679	2,4-XYLENOL	1450
106445	P-CRESOL	3747
106467	1,4-DICHLOROBENZENE	21
106489	P-CHLOROPHENOL	178
108383	1,3-DIMETHYLBENZENE(M-XYLENE)	110
108394	META-CRESOL (3-METHYLPHENOL)	3
108429	M-CHLOROANILINE	87
108430	M-CHLOROPHENOL	0
108883	METHYLBENZENE(TOLUENE)	7839
108952	PHENOL	7964
109524	PENTANOIC ACID (VALERIC ACID)	60
110656	BUTYNE-1,4-DIOL	5304
111148	HEPTANOIC ACID	34
112345	2-(2-BUTOXYETHOXY)ETHANOL	335
112345	2-(2-BUTOXYETHOXY)ETHANOL	72
112390	METHYL N-HEXADECANOATE	24
112925	1-OCTADECANOL	184
117817	DI-(2-ETHYLHEXYL)PHTHALATE	42
117817	DI-(2-ETHYLHEXYL)PHTHALATE	109
117817	DIOCTYLPHTHALATE	0
117840	DIOCTYL PHTHALATE	12161
117840	DIOCTYL PHTHALATE	23704
120127	ANTHRACENE	285
120616	DIMETHYL TEREPHTALATE	21
120729	INDOLE	255
120832	2,4-DICHLOROPHENOL	369
121335	Benzaldehyde,4-hydroxy-3-methoxy-	10
121733	1-CHLORO-3-NITROBENZENE	126
122394	DIPHENYLAMINE	12
122996	2-PHENOXYETHANOL	391
123079	PARA-ETHYLPHENOL	42

Concentrations of Confirmed Compounds
Sorted by Industrial Code and CASRN

CASRN	Compound Name	RTI CONC ng/ul (extract)
ORGANICS & PLASTICS	(Continued)	
123080	P-HYDROXY-BENZALDEHYDE	4318
123422	2-HYDROXY-2-METHYL-4-PENTANONE (DIACETONE)	< .01
124072	CAPRYLIC ACID	44
124072	CAPRYLIC ACID	222
124185	N-DECANE	50
126738	TRI-BUTYL PHOSPHATE	1131
127184	TETRACHLOROETHYLENE	2
129000	PYRENE (BENZOPHENANTHRENE)	149
129000	PYRENE	2
131113	DIMETHYL PHTHALATE	156
134963	SYRINGALDEHYDE	20
138863	LIMONENE	644
140114	BENZYL ACETATE	40
142621	N-HEXANOIC ACID	1738
142621	HEXANOIC ACID(CAPROIC ACID)	156
143077	LAURIC ACID (N-DODECANOIC ACID)	123836
203645	4,5-METHYLENE PHENANTHRENE	15
206440	FLUORANTHENE	39
259790	BIPHENYLENE	277
334485	DECANOIC ACID	1315
498022	4-HYDROXY-3-METHOXYACETOPHENONE	53
499752	CARVACROL (2-HYDROXY-4-ISOPROPYL-1-METHYLBENZENE)	158
501520	PHENYLPROPIONIC ACID	339922
529340	ALPHA-TETRALONE	58
573988	1,2-DIMETHYLNAPHTHALENE	2
575439	1,6-DIMETHYLNAPHTHALENE	< 1
576261	2,6-DIMETHYL PHENOL	604
589924	4-METHYLCYCLOHEXANONE	3
612000	1,1-DIPHENYLETHANE	8
617947	2-PHENYL-2-PROPANOL	23
620144	1-METHYL-3-ETHYLBENZENE	14
637503	PROPENYLBENZENE	< .01
706149	GAMMA-DECALACTONE	36
767599	METHYL-1-INDENE	3994
767599	1-METHYL-1H-INDENE	4
934747	1,3-DIMETHYL-5-ETHYLBENZENE	30
939275	2-ETHYLNAPHTHALENE	< 1
1490046	MENTHOL	609
1570656	4,6-DICHLORO-O-CRESOL	217
1667012	2,4,6-TRIMETHYLACETOPHENONE	16
2027170	2-ISOPROPYLNAPHTHALENE	270
25013165	BUTYLATED HYDROXY ANISOLE	7
PAINT & INK		
57103	PALMITIC ACID	5523

Concentrations of Confirmed Compounds
Sorted by Industrial Code and CASRN

PAINT & INK (Continued)

CASRN	Compound Name	RTI CONC ng/ul (extract)
58902	2,3,4,6-TETRACHLOROPHENOL	89
65850	BENZOIC ACID	14473
71432	BENZENE	30
76222	NORBORNAN-2-ONE (CAMPHOR)	124
78591	ISOPHORONE	3141
79312	ISOBUTYRIC ACID	5052
79414	METHACRYLIC ACID	5714
84742	DIBUTYL PHTHALATE	1900
85018	PHENANTHRENE	< 1
89952	O-METHYLBENZYL ALCOHOL	1106
90120	1-METHYLNAPHTHALENE	106
91203	NAPHTHALENE	13
91576	2-METHYLNAPHTHALENE	269
95476	1,2-DIMETHYLBENZENE(O-XYLENE)	2086
95636	1,2,4-TRIMETHYLBENZENE	190
98555	ALPHA-TERPINEOL	10
98555	ALPHA-TERPINEOL	189
98737	P-TERT-BUTYLBENZOIC ACID	1433
98828	ISOPROPYLBENZENE	41
98862	METHYL-PHENYL KETONE	557
99047	M-TOLUIC ACID	164
99898	P-ISOPROPYLPHENOL	121
100414	ETHYLBENZENE	21174
100425	STYRENE	2790
100516	BENZYL ALCOHOL	634
104767	2-ETHYL-1-HEXANOL	20
104767	2-ETHYL-1-HEXANOL	13
104767	2-ETHYL-1-HEXANOL	1550
106423	1,4-DIMETHYLBENZENE(P-XYLENE)	42265
107415	2-METHYL-2,4-PENTANEDIOL	281
108383	1,3-DIMETHYLBENZENE(M-XYLENE)	179
108394	META-CRESOL (3-METHYLPHENOL)	175
108678	1,3,5-TRIMETHYLBENZENE	85
108941	CYCLOHEXANONE	158
108952	PHENOL	267
109524	PENTANOIC ACID	96
110430	2-HEPTANONE	1612
111762	2-BUTOXYETHANOL	1363
111773	2-(2-METHOXYETHOXY)ETHANOL	3571
112345	2-(2-BUTOXYETHOXY)ETHANOL	35
112403	N-DODECANE	344
112403	N-DODECANE	733
112958	N-EICOSANE	17
118901	O-TOLUIC ACID	632

Concentrations of Confirmed Compounds
Sorted by Industrial Code and CASRN

CASRN	Compound Name	RTI CONC ng/ul (extract)
PAINT & INK	(Continued)	
119619	BENZOPHENONE	367
122996	2-PHENOXYETHANOL	6
124072	OCTANOIC ACID	119
126738	TRI-BUTYL PHOSPHATE	75
126738	TRI-BUTYL PHOSPHATE	9301
127184	TETRACHLOROETHYLENE	1248
131113	DIMETHYL PHTHALATE	786
135013	1,2-DIETHYLBENZENE	134
141935	1,3-DIETHYLBENZENE	15
142621	HEXANOIC ACID(CAPROIC ACID)	7825
143077	LAURIC ACID (N-DODECANOIC ACID)	434
143226	TRIETHYLENE GLYCOL N-BUTYL ETHER	3438
143248	TETRAETHYLENE GLYCOL DIMETHYL ETHER	1034
334485	DECANOIC ACID	47
488233	1,2,3,4-TETRAMETHYLBENZENE (PREHNITENE)	2267
507700	BORNEOL	51
526738	1,2,3-TRIMETHYLBENZENE	225
544638	MYRISTIC ACID	17
544763	N-HEXADECANE	1982
571619	1,5-DIMETHYLNAPHTHALENE	23
575417	1,3-DIMETHYLNAPHTHALENE	179
575417	1,3-DIMETHYLNAPHTHALENE	53
582161	2,7-DIMETHYLNAPHTHALENE	98
593453	OCTADECANE	12
611143	1-METHYL-2-ETHYLBENZENE	85
620144	M-ETHYLTOLUENE	16
622968	P-ETHYLTOLUENE	272
629505	N-TRIDECANE	1270
629594	N-TETRADECANE	856
629594	N-TETRADECANE	540
629629	N-PENTADECANE	2418
629629	N-PENTADECANE	786
629787	N-HEPTADECANE	674
629787	N-HEPTADECANE	59
629925	NONADECANE	8
829265	2,3,6-TRIMETHYLNAPHTHALENE	66
939275	2-ETHYLNAPHTHALENE	40
1074437	1-METHYL-3-N-PROPYLBENZENE	12
1120214	N-UNDECANE	770
1632731	FENCHYL ALCOHOL	255
2027170	2-ISOPROPYLNAPHTHALENE	89
2245387	2,3,5-TRIMETHYLNAPHTHALENE	27
PESTICIDES MFG.		
88062	2,4,6-TRICHLOROPHENOL	56

Concentrations of Confirmed Compounds
Sorted by Industrial Code and CASRN

CASRN	Compound Name	RTI CONC ng/ul (extract)
PESTICIDES MFG.	(Continued)	
95169	BENZOTHIAZOLE	
95476	1,2-DIMETHYLBENZENE(O-XYLENE)	292
111444	BIS(2-CHLOROETHYL)ETHER	175
117817	DI-(2-ETHYLHEXYL)PHTHALATE	5
118934	O-HYDROXYACETOPHENONE	< 1
120832	2,4-DICHLOROPHENOL	4
124185	N-DECANE	3210
127184	TETRACHLOROETHYLENE	37
143077	LAURIC ACID	1470
582161	2,7-DIMETHYLNAPHTHALENE	207
934747	5-ETHYL-M-XYLENE	300
939275	2-ETHYLNAPHTHALENE	192
1120214	N-UNDECANE	0
1127760	1-ETHYLNAPHTHALENE	77
		101
PETROLEUM REFINING		
83329	ACENAPHTHENE	
85018	PHENANTHRENE	21
86737	FLUORENE (2,3-BENZINDENE)	15
90006	ORTHO-ETHYLPHENOL	15
90120	1-METHYLNAPHTHALENE	76
91203	NAPHTHALENE	197
91576	2-METHYLNAPHTHALENE	77
95158	2,3-BENZOTHIOPENE (THIANAPHTHENE)	204
95205	2-METHYLINDOLE	36
95476	1,2-DIMETHYLBENZENE(O-XYLENE)	2
95636	1,2,4-TRIMETHYLBENZENE	13
95874	1-HYDROXY-2,5-DIMETHYLBENZENE(2,5-DIMETHYLPHENOL)	17
98737	Benzoicacid,4-(1,1-dimethylethyl)-	728
98828	ISOPROPYLBENZENE	112727
99876	P-CYMENE	32
100414	ETHYLBENZENE	< 1
100516	BENZYL ALCOHOL	11
103651	N-PROPYLBENZENE	33
105679	2,4-XYLENOL	105
106423	1,4-DIMETHYLBENZENE(P-XYLENE)	130
108383	1,3-DIMETHYLBENZENE(M-XYLENE)	761
108394	META-CRESOL (3-METHYLPHENOL)	73
108678	1,3,5-TRIMETHYLBENZENE	189
108689	3,5-XYLENOL	3
108883	TOLUENE	1221
108952	PHENOL	14
108985	BENZENETHIOL (THIOPHENOL)	5308
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Concentrations of Confirmed Compounds
Sorted by Industrial Code and CASRN

PETROLEUM REFINING (Continued)

CASRN	Compound Name	RTI CONC ng/ul (extract)
112345	2-(2-BUTOXYETHOXY)ETHANOL	60
112403	N-DODECANE	112
112958	N-EICOSANE	831
120127	ANTHRACENE	98
123079	PARA-ETHYLPHENOL	2793
124185	N-DECANE	16
127184	TETRACHLOROETHYLENE	151
128370	2,6-DI-TERT-BUTYL-4-METHYL-PHENOL	4
132650	DIBENZOTHIOPHENE	10
496117	INDANE	30
526738	1,2,3-TRIMETHYLBENZENE	53
526750	1-HYDROXY-2,3-DIMETHYLBENZENE (2,3-DIMETHYLPHENOL)	88
527606	2,4,6-TRIMETHYLPHENOL	13
527844	O-CYMENE	5
535773	M-CYMENE	64
544763	HEXADECANE (PRACTICAL)	279
571584	1,4-DIMETHYLNAPHTHALENE	56
571619	1,5-DIMETHYLNAPHTHALENE	14
575417	1,3-DIMETHYLNAPHTHALENE	148
575439	1,6-DIMETHYLNAPHTHALENE	8
576261	1-HYDROXY-2,6-DIMETHYLBENZENE(2,6-DIMETHYLPHENOL)	18
581408	2,3-DIMETHYLNAPHTHALENE	3
581420	2,6-DIMETHYLNAPHTHALENE	87
582161	2,7-DIMETHYLNAPHTHALENE	80
593453	OCTADECANE	734
593497	N-HEPTACOSANE	6
611143	1-METHYL-2-ETHYLBENZENE	15
613127	2-METHYL ANTHRACENE	12
620144	1-METHYL-3-ETHYLBENZENE	12
620177	M-ETHYLPHENOL	250
622968	1-METHYL-4-ETHYLBENZENE	15
629505	N-TRIDECANE	144
629594	N-TETRADECANE	112
629629	N-PENTADECANE	106
629787	HEPTADECANE	163
629925	NONADECANE	554
629947	N-HENEICOSANE	565
629970	N-DOCOSANE	264
629992	N-PENTACOSANE	13
630013	N-HEXACOSANE	9
630024	N-OCTACOSANE	1149
638675	N-TRICOSANE	50
829265	2,3,6-TRIMETHYLNAPHTHALENE	9
832699	1-METHYLPHENANTHRENE	79

Concentrations of Confirmed Compounds
Sorted by Industrial Code and CASRN

CASRN	Compound Name	RTI CONC ng/ul (extract)
PETROLEUM REFINING	(Continued)	
874351	5-METHYL-(2,3-DIHYDROINDENE)(5-METHYLINDAN)	14
874419	1,3-DIMETHYL-4-ETHYLBENZENE	219
883205	9-METHYLPHENANTHRENE	44
933982	3-ETHYL-O-XYLENE	5
934747	1,3-DIMETHYL-5-ETHYLBENZENE	8
939275	2-ETHYLNAPHTHALENE	402
1074175	1-METHYL-2-N-PROPYLBENZENE	14
1120214	N-UNDECANE	48
1127760	1-ETHYLNAPHTHALENE	65
1576676	3,6-DIMETHYLPHENANTHRENE	40
1576698	2,7-DIMETHYLPHENANTHRENE	7
1685821	4,6-DIMETHYLINDAN	24
1730376	1-METHYLFLUORENE	12
2027170	2-ISOPROPYLNAPHTHALENE	6
2245387	2,3,5-TRIMETHYLNAPHTHALENE	96
2847725	4-METHYLDECANE	149
4706905	1-ISOPROPYL-3,5-DIMETHYLBENZENE	2
6682719	4,7-DIMETHYLINDAN	14
6975980	2-METHYLDECANE	45
PHARMACEUTICALS		
83341	3-METHYLINDOLE	15
90437	O-PHENYLPHENOL	5
95476	O-XYLENE	27
101815	DIPHENYLMETHANE	24
103822	PHENYLACETIC ACID	62677
106423	1,4-DIMETHYLBENZENE(P-XYLENE)	135
108394	M-CRESOL	12
108429	M-CHLORDANILINE	294
108883	TOLUENE	18
112630	METHYL LINOLEATE	4
119619	BENZOPHENONE	44
143077	LAURIC ACID (N-DODECANOIC ACID)	45
492228	THIAXANTHONE	290
499752	CARVACROL (2-HYDROXY-4-ISOPROPYL-1-METHYLBENZENE)	18
501520	PHENYLPROPIONIC ACID	119151
PHOTOGRAPHIC INDUSTRIES		
88755	O-NITROPHENOL	348
94597	SAFROLE	1066
95169	BENZOTHIAZOLE	< 1
95567	O-BROMOPHENOL	24

Concentrations of Confirmed Compounds
Sorted by Industrial Code and CASRN

CASRN	Compound Name	RTI CONC ng/ul (extract)
PHOTOGRAPHIC INDUSTRIES (Continued)		
106412	P-BROMOPHENOL	137
106423	P-XYLENE	1684
108394	META-CRESOL (3-METHYLPHENOL)	23
108952	PHENOL	773
112345	2-(2-BUTOXYETHOXY)ETHANOL	3
119335	2-NITRO-P-CRESOL	51
122996	2-PHENOXYETHANOL	102
128370	(2,6-DI-TERT-BUTYL-4-METHYL PHENOL)	< 1
142621	HEXANOIC ACID(CAPROIC ACID)	5
544763	HEXADECANE	307
593453	N-OCTADECANE	4
719222	2,6-DI-TERT-BUTYL-P-BENZOQUINONE	3
872504	N-METHYL-2-PYRROLIDONE	653
4170303	2-BUTENAL (CROTONALDEHYDE)	95
PLASTICS & SYNTHETICS		
65850	BENZOIC ACID	12481
87412	PHTHALIDE	16
88993	PHTHALIC ACID	8655
92524	BIPHENYL	4
95487	O-CRESOL	< .01
99047	M-TOLUIC ACID	1410
100414	ETHYLBENZENE	< 1
101848	PHENYL ETHER	12
108952	PHENOL	34
112345	2-(2-BUTOXYETHOXY)ETHANOL	109
117817	DI-(2-ETHYLHEXYL)PHTHALATE	32
127184	TETRACHLOROETHYLENE	16
128370	2,6-DITERTIARY BUTYL-P-CRESOL (IONOL)	22
PLASTICS MFG.		
95636	1,2,4-TRIMETHYLBENZENE	46
95932	1,2,4,5-TETRAMETHYLBENZENE	2
98828	ISOPROPYLBENZENE	85
103651	N-PROPYLBENZENE	30
103651	N-PROPYLBENZENE	18
106423	P-XYLENE	364
108101	METHYL ISO-BUTYL KETONE	465
108383	1,3-DIMETHYLBENZENE(M-XYLENE)	3938
108678	1,3,5-TRIMETHYLBENZENE	227
108883	TOLUENE	99
141935	M-DIETHYLBENZENE	46

Concentrations of Confirmed Compounds
Sorted by Industrial Code and CASRN

CASRN	Compound Name	RTI CONC ng/ul (extract)
PLASTICS MFG.	(Continued)	
526738	1,2,3-TRIMETHYLBENZENE	203
611143	1-METHYL-2-ETHYLBENZENE	77
611154	O-METHYLSTYRENE	24
620144	1-METHYL-3-ETHYLBENZENE	191
622968	1-METHYL-4-ETHYLBENZENE	388
874419	1,3-DIMETHYL-4-ETHYLBENZENE	42
934747	1,3-DIMETHYL-5-ETHYLBENZENE	6
PORCELAIN/ENAMELING		
95169	BENZOTHIAZOLE	5
112050	NONANOIC ACID	28
143077	LAURIC ACID (N-DODECANOIC ACID)	69
PRINTING & PUBLISHING		
57103	PALMITIC ACID	1723
65850	BENZOIC ACID	1228
70553	P-TOLUENESULPHONAMIDE	19841
71432	BENZENE	523
84742	DIBUTYL PHTHALATE	25
90120	1-METHYLNAPHTHALENE	< .01
90153	1-NAPHTHOL	2816
91598	2-AMINONAPHTHALENE	9150
93981	BENZANILIDE	48
95476	O-XYLENE	23
95534	O-TOLUIDINE	19
95636	1,2,4-TRIMETHYLBENZENE	57
98836	ALPHA-METHYLSTYRENE	184
98862	METHYL-PHENYL KETONE	1570
104767	2-ETHYL-1-HEXANOL	9
106423	1,4-DIMETHYLBENZENE(P-XYLENE)	25
107926	N-BUTANOIC ACID(BUTYRIC ACID)	66543
108101	4 METHYL-PENTANONE 2	1125
109524	PENTANOIC ACID (VALERIC ACID)	522
111762	2-BUTOXYETHANOL	74179
111900	2-(2-ETHOXYETHOXY) ETHANOL	52189
112345	2-(2-BUTOXYETHOXY)ETHANOL	47933
112403	DODECANE	30
112721	1-TETRADECANOL	49
112958	N-EICOSANE	96
120821	1,2,4 TRICHLOROBENZENE	186
124072	OCTANOIC ACID	279
124185	N-DECANE	1

Concentrations of Confirmed Compounds
Sorted by Industrial Code and CASRN

CASRN	Compound Name	RTI CONC ng/ul (extract)
PRINTING & PUBLISHING (Continued)		
126738	TRI-BUTYL PHOSPHATE	32
127184	TETRACHLOROETHYLENE	39
135193	2-NAPHTHOL	56
143226	TRIETHYLENE GLYCOL N-BUTYL ETHER	3868
526738	1,2,3-TRIMETHYLBENZENE	120
544638	TETRADECANOIC ACID	23
544763	HEXADECANE (PRACTICAL)	104
571619	1,5-DIMETHYLNAPHTHALENE	119
582161	2,7-DIMETHYLNAPHTHALENE	86
593453	OCTADECANE	656
620144	1-METHYL-3-ETHYLBENZENE	205
629505	N-TRIDECANE	72
629629	N-PENTADECANE	113
629787	N-HEPTADECANE	42
629925	NONADECANE	14
643583	2-METHYLBIPHENYL	5
1120214	N-UNDECANE	14
2245387	2,3,5-TRIMETHYLNAPHTHALENE	6
PUBLIC OWNED TREAT WORKS		
50328	3,4-BENZPYRENE	73
57103	PALMITIC ACID	28693
57103	PALMITIC ACID	1888
57114	STEARIC ACID	261
58082	CAFFEIN	47
58082	CAFFEIN	48
58082	CAFFEINE	46
60571	DIELDRIN	4
62533	ANILINE	85
78400	TRIETHYL PHOSPHATE (ETHYL PHOSPHATE)	4
79094	PROPANOIC ACID(PROPIONIC ACID)	5911
83329	ACENAPHTHENE	22
83330	1-INDANONE	7
83341	3-METHYLINDOLE	69
84662	DIETHYL PHTHALATE	15
84742	BUTYL PHTHALATE	2
86748	CARBAZOLE	66
87616	1,2,3-TRICHLOROBENZENE	8
88697	ORTHO-ISOPROPYLPHENOL (ORTHO-CUMENOL)	112
90006	O-ETHYLPHENOL	105
90120	1-METHYL NAPHTHALENE	96
90131	1-CHLORONAPTHALENE	24
90131	1-CHLORONAPTHALENE	22

Concentrations of Confirmed Compounds
Sorted by Industrial Code and CASRN

PUBLIC OWNED TREAT WORKS (Continued)

CASRN	Compound Name	RTI CONC ng/ul (extract)
90437	1-HYDROXY-2-PHENYLBENZENE	5
91203	NAPHTHALENE	80
91225	QUINOLINE (1-BENZAZINE)	6
91576	2-METHYLNAPHTHALENE	379
95205	2-METHYLINDOLE	3
95476	1,2-DIMETHYLBENZENE(O-XYLENE)	419
95487	ORTHO-CRESOL (2-METHYLPHENOL)	217
95501	O-DICHLOROBENZENE	2
95534	O-TOLUIDINE	40
95636	1,2,4-TRIMETHYLBENZENE	350
95761	3,4-DICHLOROANILINE	25
95874	1-HYDROXY-2,5-DIMETHYLBENZENE(2,5-DIMETHYLPHENOL)	255
95932	1,2,4,5-TETRAMETHYLBENZENE	< .01
96764	2,4-DI-TERT-BUTYLPHENOL	3
96764	2,4-DI-TERT-BUTYLPHENOL	6
98000	FURFURYL ALCOHOL	992
98544	P-TERT-BUTYLPHENOL (IN METHANOL)	24
98555	ALPHA-TERPINEOL	78
98828	ISOPROPYLBENZENE	4
98828	ISOPROPYLBENZENE	< 1
99047	M-TOLUIC ACID	998
99865	ALPHA TERPINENE	2
99898	P-ISOPROPYLPHENOL	6
100414	ETHYLBENZENE	279
100516	BENZYL ALCOHOL	11
100696	2-VINYLPYRIDINE	68
103651	N-PROPYLBENZENE	22
103822	PHENYLACETIC ACID	110
105679	2,4-XYLENOL	59
106423	1,4-DIMETHYLBENZENE(P-XYLENE)	401
106445	P-CRESOL	539
106467	1,4-DICHLOROBENZENE	28
106934	1,2-DIBROMOETHANE	19
107926	N-BUTANOIC ACID(BUTYRIC ACID)	401
108383	1,3-DIMETHYLBENZENE(M-XYLENE)	12
108394	META-CRESOL (3-METHYLPHENOL)	747
108394	META-CRESOL (3-METHYLPHENOL)	6001
108678	1,3,5-TRIMETHYLBENZENE	34
108689	3,5-DIMETHYL PHENOL	10
108703	1,3,5-TRICHLOROBENZENE	2
108883	METHYLBENZENE (TOLUENE)	786
108952	PHENOL	2450
109068	2-METHYLPYRIDINE	9
109524	VALERIC ACID	55

Concentrations of Confirmed Compounds Sorted by Industrial Code and CASRN

PUBLIC OWNED TREAT WORKS (Continued)

CASRN	Compound Name	RTI CONC ng/ul (extract)
111148	HEPTANOIC ACID	65
111762	2-N-BUTOXYETHANOL	651
111900	2-(2-ETHOXYETHOXY) ETHANOL	2
112050	NONANOIC ACID	13
112345	2-(2-BUTOXYETHOXY)ETHANOL	539
112403	N-DODECANE	7
112721	TETRADECANOL	< 1
112958	N-EICOSANE	44
117817	DI-(2-ETHYLHEXYL)PHTHALATE	4
117817	DI-(2-ETHYLHEXYL)PHTHALATE	< 1
120127	ANTHRACENE	< .01
120729	INDOLE	154
123079	P-ETHYLPHENOL	91
123637	PARALDEHYDE	2
123911	1,4-DIOXANE	575
124072	CAPRYLIC ACID	116
124185	N-DECANE	67
127184	TETRACHLOROETHYLENE	13
127184	TETRACHLOROETHYLENE	16
129000	PYRENE (BENZOPHENANTHRENE)	1
132649	DIBENZOFURAN	< 1
142621	HEXANOIC ACID(CAPROIC ACID)	21
143077	LAURIC ACID	209
206440	FLUORANTHENE (1,2-BENZACENAPTHENE)	1
218019	CHRYSENE	13
334485	DECANOIC ACID	33
475207	LONGIFOLENE	23
496786	2,4,5-TRIMETHYLPHENOL	55
499069	3,5-DIMETHYL-BENZOIC ACID	286
526738	1,2,3-TRIMETHYLBENZENE	43
526750	2,3-DIMETHYLPHENOL	23
527548	3,4,5-TRIMETHYLPHENOL	21
527606	2,4,6-TRIMETHYLPHENOL	3
535773	1-METHYL-3-ISOPROPYLBENZENE	6
541731	1,3-DICHLOROBENZENE	4
544638	MYRISTIC ACID	198
544638	MYRISTIC ACID	1083
544763	N-HEXADECANE	41
571584	1,4-DIMETHYLNAPHTHALENE	20
575417	1,3-DIMETHYLNAPHTHALENE	46
575439	1,6-DIMETHYLNAPHTHALENE	10
576261	2,6-DIMETHYL PHENOL	3
581408	2,3-DIMETHYLNAPHTHALENE	0
582161	2,7-DIMETHYLNAPHTHALENE	42

Concentrations of Confirmed Compounds
Sorted by Industrial Code and CASRN

CASRN	Compound Name	RTI CONC ng/ul (extract)
PUBLIC OWNED TREAT WORKS (Continued)		
593453	OCTADECANE	54
611143	1-METHYL-2-ETHYLBENZENE	40
613127	2-METHYL ANTHRACENE	2
614960	5-METHYLINDOLE	600
619045	3,4-DIMETHYL-BENZOIC ACID	169
620144	1-METHYL-3-ETHYLBENZENE	27
620177	META-ETHYLPHENOL	289
622968	P-ETHYLTOLUENE	33
622968	P-ETHYLTOLUENE	7
624920	DIMETHYLDISULFIDE	11
629505	TRIDECANE	107
629594	N-TETRADECANE	77
629629	PENTADECANE	58
629787	N-HEPTADECANE	63
629925	NONADECANE	22
638539	TRIDECANOIC ACID	49
697825	2,3,5-TRIMETHYLPHENOL	128
829265	2,3,6-TRIMETHYLNAPHTHALENE	8
939275	2-ETHYLNAPHTHALENE	11
1074175	1-METHYL-2-N-PROPYLBENZENE	43
1685821	4,6-DIMETHYLINDAN	12
36653824	N-HEXADECANOL	322
PULP & PAPER		
54115	NICOTINE	20
57114	STEARIC ACID	458
58082	CAFFEIN	262
65850	BENZOIC ACID	741
67685	DIMETHYL SULPHOXIDE	1
67710	DIMETHYL SULFONE	273
67710	DIMETHYL SULFONE	11
71556	1,1,1-TRICHLOROETHANE	80
78591	3,5,5-TRIMETHYL-2-CYCLOHEXENONE(ISOPHORONE)	14
80568	ALFA-PINENE	9
84662	ETHYL PHTHALATE	21
84742	BUTYL PHTHALATE	31
84742	DIBUTYL PHTHALATE	8
85018	PHENANTHRENE	1
85687	BUTYL BENZYL PHTHALATE	9
86817	3,4,5-TRIMETHOXYBENZALDEHYDE	3
89816	PIPERITONE	9
90051	ORTHO-METHOXYPHENOL	1886
90120	1-METHYL NAPHTHALENE	3

Concentrations of Confirmed Compounds
Sorted by Industrial Code and CASRN

PULP & PAPER (Continued)

CASRN	Compound Name	RTI CONC ng/ul (extract)
91167	1,2-DIMETHOXYBENZENE (VERATROLE)	3
91203	NAPHTHALENE	2
91576	2-METHYLNAPHTHALENE	28
95476	1,2-DIMETHYLBENZENE(O-XYLENE)	< .01
95954	2,4,5-TRICHLOROPHENOL	67
97530	EUGENOL	1043
97541	2-METHOXY-4-(PROP-2-ENYL)-PHENOL (ISOEUGENOL)	209
98000	FURFURYL ALCOHOL	115
98011	FURFURAL	1283
98555	ALPHA-TERPINEOL	278
98862	ACETOPHENONE	128
99876	P-CYMENE	< .01
100414	ETHYLBENZENE	2
100425	STYRENE	17
100516	BENZYL ALCOHOL	255
103822	PHENYLACETIC ACID	61
108952	PHENOL	17
109524	PENTANOIC ACID (VALERIC ACID)	7
111762	2-BUTOXYETHANOL	226
111900	DIETHYLENE GLYCOL MONOETHYL ETHER	40
112345	2-(2-BUTOXYETHOXY)ETHANOL	34
112958	N-EICOSANE	26
117817	DI-(2-ETHYLHEXYL)PHTHALATE	10
120127	ANTHRACENE	7
120832	2,4-DICHLOROPHENOL	7
121335	VANILLIN	600
123795	DIOCTYL ADIPATE	21
124072	OCTANOIC ACID	399
126738	TRI-BUTYL PHOSPHATE	7
127184	TETRACHLOROETHYLENE	110
129000	PYRENE (BENZOPHENANTHRENE)	3
132650	DIBENZOTHIOPHENE	< 1
134963	SYRINGALDEHYDE	27
140670	P-ALLYLANISOLE	< 1
142507	NEROLIDOL	40
142621	HEXANOIC ACID(CAPROIC ACID)	723
143077	LAURIC ACID (N-DODECANOIC ACID)	92
150765	P-METHOXYPHENOL	11
306081	4-HYDROXY-3-METHOXY-PHENYLACETIC ACID	2588
334485	CAPRIC ACID	133
498022	ACETOVANILLON (4-HYDROXY-3-METHOXYACETOPHENONE)	47
499752	P-CYMEN-ALPHA-OL	2
501520	PHENYLPROPIONIC ACID	195
507700	1-BORNEOL	102

Concentrations of Confirmed Compounds
Sorted by Industrial Code and CASRN

CASRN	Compound Name	RTI CONC ng/ul (extract)
PULP & PAPER	(Continued)	
507700	BORNEOL	10
535773	M-CYMENE	2
535808	M-CHLOROBENZOIC ACID	17
544763	N-HEXADECANE	72
562743	TERPINENE-4-OL	7
562743	TERPINENE-4-OL	57
571619	1,5-DIMETHYLNAPHTHALENE	< 1
586629	TERPINOLENE	28
593453	OCTADECANE	63
593497	N-HEPTACOSANE	7
615225	2(METHYLTHIO)BENZOTHIAZOLE	4
622968	P-ETHYLTOLUENE	< .01
624920	2,3-DITHIABUTANE	14
629505	N-TRIDECANE	39
629594	N-TETRADECANE	53
629629	N-PENTADECANE	66
629787	N-HEPTADECANE	84
629992	N-PENTACOSANE	7
634366	1,2,3-TRIMETHOXYBENZENE	4
638675	N-TRICOSANE	49
638686	TRIACONTANE	5
1195795	FENCHONE	75
1632731	FENCHYL ALCOHOL	2
2078548	2,6-DIISOPROPYL PHENOL	3
2478388	ACETOSYRINGONE	38
2758181	3-METHYLCYCLOPENT-2-ENE-1-ONE	42
2758181	3-METHYLCYCLOPENT-2-ENE-1-ONE	4
2896608	4-ETHYLSORCINOL	5
6628188	1,2-BIS(METHYLMERCAPTO)ETHANE	2
13466789	DELTA-3-CARENE	13
13466789	3-CARENE	16
18172673	BETA PINENE	3
18172673	BETA PINENE	4
RUBBER PROCESSING		
62533	ANILINE	68656
71432	BENZENE	354
79925	CAMPHENE	396
83330	INDAN-1-ONE	19
88697	O-ISOPROPYLPHENOL	95
91203	NAPHTHALENE	74
91225	QUINOLINE	95
92842	PHENOTHIAZINE	29441

Concentrations of Confirmed Compounds
Sorted by Industrial Code and CASRN

RUBBER PROCESSING (Continued)

CASRN	Compound Name	RTI CONC ng/ul (extract)
95169	BENZOTHIAZOLE	535
95476	1,2-DIMETHYLBENZENE(O-XYLENE)	814
95738	2,4-DICHLOROTOLUENE	1241
95750	3,4-DICHLOROTOLUENE	203
95932	1,2,4,5-TETRAMETHYLBENZENE	110
96093	EPOXYETHYL BENZENE (STYRENE OXIDE)	173
98544	P-TERT-BUTYLPHENOL (IN METHANOL)	6
98555	ALPHA-TERPINEOL	1993
98828	ISOPROPYLBENZENE	596
99876	1-METHYL-4-ISOPROPYLBENZENE	4296
100414	ETHYL BENZENE	2378
100425	STYRENE	82
100425	STYRENE	855
100696	2-VINYLPYRIDINE	209
100710	2-ETHYLPYRIDINE	23
101848	PHENYL ETHER	18
104767	2-ETHYL-1-HEXANOL	284
105679	2,4-DIMETHYL PHENOL	70
106445	PARA-CRESOL (4-METHYLPHENOL)	140
108383	M-XYLENE	1222
108689	3,5-XYLENOL	46
108883	TOLUENE	27
111762	2-BUTOXYETHANOL	55
112345	2-(2-BUTOXYETHOXY) ETHANOL	84
112345	2-(2-BUTOXYETHOXY) ETHANOL	30
117817	DI-(2-ETHYLHEXYL)PHTHALATE	123
120752	2-METHYLBENZOTHIAZOLE	31
122394	DIPHENYLAMINE	2142
122394	DIPHENYLAMINE	1233
123079	P-ETHYLPHENOL	360
123422	2-HYDROXY-2-METHYL-4-PENTANONE (DIACETONE)	4
124072	OCTANOIC ACID	1511
127184	TETRACHLOROETHYLENE	3
128370	2,6-DITERTIARY BUTYL-P-CRESOL (IONOL)	76
138863	LIMONENE	14947
142621	HEXANOIC ACID(CAPROIC ACID)	736
147477	2,2,4-TRIMETHYLDIHYDROQUINOLINE	1058
147477	2,2,4-TRIMETHYLDIHYDROQUINOLINE	501
147820	2,4,6-TRIBROMOANILINE	< 1
300572	3-PHENYL-1-PROPENE (ALLYLBENZENE)	28
470826	1,8-CINEOLE	871
488233	1,2,3,4-TETRAMETHYLBENZENE (PREHNITENE)	8
507700	BORNEOL	374
527537	1,2,3,5-TETRAMETHYLBENZENE	72

Concentrations of Confirmed Compounds
Sorted by Industrial Code and CASRN

CASRN	Compound Name	RTI CONC ng/ul (extract)
RUBBER PROCESSING	(Continued)	
544763	N-HEXADECANE	34
593453	OCTADECANE	99
611143	1-METHYL-2-ETHYLBENZENE	370
615225	2(METHYLTHIO)BENZOTHIAZOLE	11
620144	1-METHYL-3-ETHYLBENZENE	928
622968	1-METHYL-4-ETHYLBENZENE	10
622968	1-METHYL-4-ETHYLBENZENE	38
629629	N-PENTADECANE	13
629787	HEPTADECANE	64
697825	2,3,5-TRIMETHYLPHENOL	60
874419	1,3-DIMETHYL-4-ETHYLBENZENE	62
882337	DIPHENYL DISULFIDE	100
1195795	FENCHONE	260
1632731	FENCHYL ALCOHOL	4034
4706905	1-ISOPROPYL-3,5-DIMETHYLBENZENE	1
13466789	3-CARENE	874
RUM INDUSTRY		
60128	2-PHENYL ETHANOL	4294
90051	O-METHOXYPHENOL	59
98000	FURFURYL ALCOHOL	519
98011	2-FURALDEHYDE	5665
100516	BENZYL ALCOHOL	111
104767	2-ETHYL-1-HEXANOL	72
108509	2,6-DIMETHYLPYRAZINE	154
108952	PHENOL	51
110838	CYCLOHEXENE	1476
112345	2-(2-BUTOXYETHOXY) ETHANOL	147
122974	3-PHENYLPROPANOL	32
124061	ETHYL MYRISTATE	2022
496162	2,3-DIHYDROBENZOFURAN	204
498022	ACETOVANILLON (4-HYDROXY-3-METHOXYACETOPHENONE)	32
628977	ETHYL PALMITATE	3811
1072839	2-ACETYLPYRROLE	608
2033898	3,4-DIMETHOXYPHENOL	580
SOAPS & DETERGENTS		
92524	DIPHENYL	14
101848	DIPHENYL ETHER	30
101848	DIPHENYLETHER	38
106332	ETHYL LAURATE	50
106332	ETHYL LAURATE	21

Concentrations of Confirmed Compounds
Sorted by Industrial Code and CASRN

CASRN	Compound Name	RTI CONC ng/ul (extract)
SOAPS & DETERGENTS (Continued)		
110429	METHYL CAPRATE	10
111115	OCTANOIC ACID-METHYL ESTER	6
111820	METHYL LAURATE	76
112129	2-UNDECANONE	453
112129	2-UNDECANONE	336
112618	METHYL STEARATE	334
124061	ETHYL MYRISTATE	20
124107	METHYL MYRISTATE	46
127184	TETRACHLOROETHYLENE	69
143077	LAURIC ACID	14979
334485	DECANOIC ACID	8822
593088	2-TRIDECANONE	79
593088	2-TRIDECANONE	40
629594	N-TETRADECANE	3
629629	N-PENTADECANE	42
821556	METHYL HEPTYL KETONE	42
STEAM ELECTRIC		
84695	DIISOBUTYL PHTHALATE	< 1
84742	N-BUTYL O-PHTHALATE	18
106423	1,4-DIMETHYLBENZENE(P-XYLENE)	< 1
117817	DI-(2-ETHYLHEXYL)PHTHALATE	< 1
544763	HEXADECANE (PRACTICAL)	< 1
593453	OCTADECANE	< 1
629629	N-PENTADECANE	< 1
629787	HEPTADECANE	< 1
SYNFUELS		
60128	2-PHENYL ETHANOL	99
98000	FURFURYL ALCOHOL	113
106445	P-CRESOL	241
108952	PHENOL	29
120729	INDOLE	179
123513	3-METHYL-1-BUTANOL	43
7683649	SQUALENE	52
TEXTILE MILLS		
57103	PALMITIC ACID	153
57885	CHOLESTEROL	1
65850	BENZOIC ACID	2054
76222	CAMPHOR	33

Concentrations of Confirmed Compounds
Sorted by Industrial Code and CASRN

TEXTILE MILLS (Continued)

CASRN	Compound Name	RTI CONC ng/ul (extract)
79094	PROPIONIC ACID	38144
79312	ISOBUTYRIC ACID	784
87616	1,2,3-TRICHLOROBENZENE	21
92524	BIPHENYL	23
95487	ORTHO-CRESOL (2-METHYLPHENOL)	16
95636	1,2,4-TRIMETHYLBENZENE	160
98828	ISOPROPYLBENZENE	186
99047	M-TOLUIC ACID	204
100414	ETHYLBENZENE	64
103651	N-PROPYLBENZENE	218
103822	PHENYLACETIC ACID	7
104767	2-ETHYL-1-HEXANOL	217
104767	2-ETHYL-1-HEXANOL	125
106423	P-XYLENE	36
106445	PARA-CRESOL (4-METHYLPHENOL)	208
107415	2-METHYL-2,4-PENTANEDIOL	51
107926	N-BUTYRIC ACID	2072
108383	1,3-DIMETHYLBENZENE(M-XYLENE)	762
108394	META-CRESOL (3-METHYLPHENOL)	101
108678	1,3,5-TRIMETHYLBENZENE	266
108952	PHENOL	48
109524	PENTANOIC ACID (VALERIC ACID)	82
111762	2-BUTOXYETHANOL	71
112345	2-(2-BUTOXYETHOXY) ETHANOL	236
112345	2-(2-BUTOXYETHOXY)ETHANOL	52
112403	N-DODECANE	262
112538	DODECANOL	9
112721	1-TETRADECANOL	36
112925	1-OCTADECANOL	94
120821	1,2,4 TRICHLOROBENZENE	80
124185	N-DECANE	34
135988	SEC-BUTYLBENZENE	105
141935	M-DIETHYLBENZENE	238
143077	LAURIC ACID (N-DODECANOIC ACID)	39
507700	BORNEOL	66
526738	1,2,3-TRIMETHYLBENZENE	16
526738	1,2,3-TRIMETHYLBENZENE	15
527844	O-CYMENE	265
544638	MYRISTIC ACID	4
611143	O-ETHYLTOLUENE	1849
620144	1-METHYL-3-ETHYLBENZENE	13
622968	P-ETHYLTOLUENE	50
629732	1-HEXADECENE	19
629992	N-PENTACOSANE	38

Concentrations of Confirmed Compounds
Sorted by Industrial Code and CASRN

CASRN	Compound Name	RTI CONC ng/ul (extract)
TEXTILE MILLS	(Continued)	
638675	N-TRICOSANE	75
1074175	1-METHYL-2-N-PROPYLBENZENE	4
36653824	1-HEXADECANOL	21
TIMBER PRODUCTS		
56553	1,2-BENZANTHRACENE	5
60128	2-PHENYL ETHANOL	11
62533	ANILINE	644
65850	BENZOIC ACID	12
69727	SALICYLIC ACID	3687
71432	BENZENE	3
76222	CAMPHOR	8
83329	ACENAPHTHENE	7294
84651	ANTHRAQUINONE	120
85018	PHENANTHRENE	3802
86737	FLUORENE	2675
86748	CARBAZOLE	1083
90051	ORTHO-METHOXYPHENOL	100
90120	1-METHYLNAPHTHALENE	98
90120	1-METHYL NAPHTHALENE	754
91203	NAPHTHALENE	184
91203	NAPHTHALENE	3885
91225	QUINOLINE	5758
91576	2-METHYLNAPHTHALENE	612
91576	2-METHYLNAPTHALENE	2919
92524	BIPHENYL	522
95136	INDENE	8252
95158	BENZO(B)THIOPHENE	5
95487	ORTHO-CRESOL (2-METHYLPHENOL)	549
95636	1,2,4-TRIMETHYLBENZENE	77
98011	FURFURAL	314
98555	ALPHA-TERPINEOL	45
100414	ETHYLBENZENE	47
100470	BENZONITRILE (CYANOBENZENE)	877
104767	2-ETHYL-1-HEXANOL	521
105135	P-ANISYLALCOHOL	65
106445	PARA-CRESOL (4-METHYLPHENOL)	770
107926	N-BUTANOIC ACID(BUTYRIC ACID)	22213
108383	M-XYLENE	21
108394	META-CRESOL (3-METHYLPHENOL)	1685
108689	3,5-XYLENOL	462
108758	2,4,6-TRIMETHYL PYRIDINE	337
108952	PHENOL	1018

Concentrations of Confirmed Compounds
Sorted by Industrial Code and CASRN

TIMBER PRODUCTS (Continued)

CASRN	Compound Name	RTI CONC ng/ul (extract)
109068	2-METHYLPYRIDINE	156
110861	PYRIDINE	711
112345	2-(2-BUTOXYETHOXY)ETHANOL	7
112390	METHYL PALMITATE	62
112403	N-DODECANE	165
112958	N-EICOSANE	47
119653	ISOQUINOLINE	5739
120127	ANTHRACENE	699
120729	INDOLE	474
121335	VANILLIN	1744
122974	3-PHENYLPROPANOL	6
123079	PARA-ETHYLPHENOL	362
127184	TETRACHLOROETHYLENE	1073
132649	DIBENZOFURAN	113
132650	DIBENZOTHIOPHENE	23
132650	DIBENZO(BD)THIOPHENE(DIPHENYLENE SULFIDE)	32
134963	SYRINGALDEHYDE (4-HYDROXY-3,5-DIMETHOXYBENZALDEHYDE)	83
135193	2-NAPHTHOL	559
198550	PERYLENE	143
203645	4,5-METHYLENEPHENANTHRENE	29
206440	FLUORANTHENE	448
207089	11,12-BENZFLUORANTHENE	468
208968	ACENAPHTHALENE	86
217594	TRIPHENYLENE	28
218019	CHRYSENE	8449
243174	2,3 BENZOFLUORENE	36
259790	BIPHENYLENE	522
271896	BENZOFURAN	88
306081	Benzeneaceticacid,4-hydroxy-3-methoxy-	8304
496117	2,3-DIHYDROINDENE (INDAN)	9
496786	2,4,5-TRIMETHYLPHENOL	1335
498022	ACETOVANILLONE	30
501520	Benzenepropanoicacid	29598
526738	1,2,3-TRIMETHYLBENZENE	23
526738	1,2,3-TRIMETHYLBENZENE	9
526750	1-HYDROXY-2,3-DIMETHYLBENZENE(2,3-DIMETHYLPHENOL)	12244
544763	N-HEXADECANE	781
571584	1,4-DIMETHYLNAPHTHALENE	7
571619	1,5-DIMETHYLNAPHTHALENE	91
581420	2,6-DIMETHYLNAPHTHALENE	3070
582161	2,7-DIMETHYLNAPHTHALENE	17
593453	OCTADECANE	155
593497	N-HEPTACOSANE	517
605027	ALPHA-PHENYLNAPHTHALENE	6

Concentrations of Confirmed Compounds
Sorted by Industrial Code and CASRN

CASRN	Compound Name	RTI CONC ng/ul (extract)
TIMBER PRODUCTS	(Continued)	
612942	2-PHENYLNAPHTHALENE	367
612942	2-PHENYLNAPHTHALENE	6976
618451	META-ISOPROPYLPHENOL	25
621829	CINNAMIC ACID	337
629505	N-TRIDECANE	203
629594	TETRADECANE	313
629629	N-PENTADECANE	600
629925	NONADECANE	781
629970	Docosane	120
638675	N-TRICOSANE	2
829265	2,3,6-TRIMETHYLNAPHTHALENE	11
832699	1-METHYLPHENANTHRENE	4139
883205	9-METHYLPHENANTHRENE	48
939275	2-ETHYLNAPHTHALENE	1320
1127760	1-ETHYLNAPHTHALENE	78
1632731	FENCHYL ALCOHOL	6
1685821	4,6-DIMETHYLINDAN	12
1921706	2,6,10,14-TETRAMETHYL PENTADECANE	89
2531842	2-METHYLPHENANTHRENE	10
3442782	2-METHYLPYRENE	731
6682719	4,7-DIMETHYLINDAN	15
20324338	TRIPROPYLENE GLYCOL METHYL ETHER	14
TRANSPORTATION EQUIPMENT		
59507	4-CHLORO-M-CRESOL	249
65850	BENZOIC ACID	639
79005	1,1,2-TRICHLOROETHANE	338
79016	TRICHLOROETHYLENE	35
91203	NAPHTHALENE	28
94597	SAFROLE	19
98862	ACETOPHENONE	106
108883	TOLUENE	346
111762	2-N-BUTOXYETHANOL	191359
112254	2-HEXYLOXYETHANOL	10141
127184	TETRACHLOROETHYLENE	2878
544763	N-HEXADECANE	37
617947	2-PHENYL-2-PROPANOL	2513
629787	N-HEPTADECANE	45

Appendix F

Compounds sorted by Percent Indicated, Percent Confirmed, and CASRN

Occurrences to Confirm	Compound name	CASRN	RTI Tentative Ident. %IND	Confirmations %CONF
3	BENZAMIDE	55210	0.	0.
1	9,10-DIMETHYL-1,2-BENZANTHRACENE	57976	0.	0.
1	GAMMA-1,2,3,4,5,6-HEXACHLOROCYCLOHE	58899	0.	0.
1	P-NITROBENZOIC ACID	62237	0.	0.
1	3,5-DIMETHYLPYRAZOLE	67516	0.	0.
1	BARBITURIC ACID	67527	0.	0.
1	2-MERCAPTOETHANOIC ACID	68111	0.	0.
2	1,2,3,4,10,10-HEXACHLORO-6,7-EPOXY-	72208	0.	0.
2	P-CHLOROBENZOIC	74113	0.	0.
1	2,2-DICHLOROPROPIONIC ACID	75990	0.	0.
1	HEXACHLOROCYCLOPENTADIENE	77474	0.	0.
1	Phenol,4,4'-(1-methylethylidene)bis	80057	0.	0.
1	PHTHALIMIDE	85416	0.	0.
1	1-(CHLOROMETHYL)NAPHTHALENE	86522	0.	0.
1	2-HYDROXYDIBENZOFURAN	86771	0.	0.
1	1,3-HEXACHLOROBUTADIENE	87683	0.	0.
1	2-CHLORONAPHTHALENE	91587	0.	0.
1	COUMARIN	91645	0.	0.
1	PHENAZINE	92820	0.	0.
2	XANTHENE	92831	0.	0.
1	2,4-DICHLOROPHENOXYACETIC ACID	94757	0.	0.
2	BENZOTRIAZOLE	95147	0.	0.
2	1,2,3-TRICHLOROPROPANE	96184	0.	0.
1	2(3H)-Furanone,dihydro-	96480	0.	0.
1	CYCLOHEXANECARBOXYLIC ACID	98895	0.	0.
1	Benzenamine,2-methyl-5-nitro-	99558	0.	0.
4	Benzoicacid,4-methyl-	99945	0.	0.
5	P-NITROPHENOL	100027	0.	0.
1	P-NITROPHENETOLE	100298	0.	0.
2	BENZYL CHLORIDE	100447	0.	0.
1	PHENYLMERCURIC CHLORIDE	100561	0.	0.
2	N-METHYLANILINE	100618	0.	0.
1	1,3,5-TRIETHYLBENZENE	102250	0.	0.
1	ETHYL CINNAMATE	103366	0.	0.
1	DIBENZYLETHER	103504	0.	0.
1	ACETANILIDE	103844	0.	0.
1	Benzene,butyl-	104518	0.	0.
1	2-(2-PHENOXYETHOXY) ETHANOL	104687	0.	0.
1	P-TOLUALDEHYDE	104870	0.	0.
1	ETHYL N-OCTANOATE	106321	0.	0.
2	P-BENZOQUINONE	106514	0.	0.
1	1-METHYL-3-CHLOROBENZENE	108418	0.	0.
1	2,6-DIMETHYLPYRIDINE	108485	0.	0.
1	M-DIVINYLBENZENE	108576	0.	0.
1	CYCLOHEXYL AMINE	108918	0.	0.
3	CYCLOHEXANOL	108930	0.	0.
1	PYRROLE	109977	0.	0.
1	ETHYL DECANOATE	110383	0.	0.
1	2-OCTANONE	111137	0.	0.
1	HEPTANAL	111717	0.	0.
3	1-OCTANOL	111875	0.	0.

Compounds sorted by Percent Indicated, Percent Confirmed, and CASRN

Occurrences to Confirm	Compound name	CASRN	RTI Tentative Ident. %IND	Confirmations %CONF
3	1-DECANOL	112301	0.	0.
1	N-DECANAL	112312	0.	0.
9	UNDECANOIC ACID	112378	0.	0.
1	1-DODECENE	112414	0.	0.
1	Ethanol,2-[2-(2-ethoxyethoxy)ethoxy	112505	0.	0.
4	OLEIC ACID	112801	0.	0.
1	DOCOSANOIC ACID	112856	0.	0.
2	1-OCTADECENE	112889	0.	0.
1	HEXACHLOROBENZENE	118741	0.	0.
3	O-CHLOROBENZOIC ACID	118912	0.	0.
1	O-AMINOBENZOIC ACID	118923	0.	0.
6	3-METHOXY-4-HYDROXYBENZOIC ACID	121346	0.	0.
1	DIMETHYLANILINE	121697	0.	0.
1	CHLORO-4,6-BIS(ETHYLAMINO)-S-TRIAZI	122349	0.	0.
1	PHENOXYACETIC ACID	122598	0.	0.
1	PHENYL ACETATE	122792	0.	0.
1	P-ANISALDEHYDE	123115	0.	0.
1	2,5-DIMETHYLPYRAZINE	123320	0.	0.
1	ISOBORNEOL	124765	0.	0.
1	ORTHO-METHYL THIOPHENOL	137064	0.	0.
2	SORBALDEHYDE	142836	0.	0.
1	1-NONANOL	143088	0.	0.
1	8-HYDROXYQUINOLINE	148243	0.	0.
1	Hexanoicacid,2-ethyl-	149575	0.	0.
1	2,3-O-PHENYLENEPYRENE	193395	0.	0.
1	3,4-BENZOPHENANTHRENE	195197	0.	0.
1	PHENANTHRIDINE	229878	0.	0.
1	1,2-BENZOFLUORENE	238846	0.	0.
1	DIBENZO-P-DIOXIN	262124	0.	0.
1	1,2,4-TRITHIOLANE	289167	0.	0.
2	CYCLODODECANE	294622	0.	0.
1	ALDRIN	309002	0.	0.
1	DIAZINON	333415	0.	0.
1	Benzenesulfonylfluoride,4-methyl-	455163	0.	0.
1	ISOCARBOSTYRIL	491305	0.	0.
1	1-Propanol,3-(methylthio)-	505102	0.	0.
1	ARACHIDIC ACID	506309	0.	0.
1	2,3-BUTANEDIOL	513859	0.	0.
1	1,3-DICHLOROACETONE	534076	0.	0.
1	N-BENZYLIDENEPHENYLAMINE	538512	0.	0.
1	O-METHYLACETOPHENONE	577162	0.	0.
2	ACRIDONE	578950	0.	0.
1	Benzene,nitroso-	586969	0.	0.
1	STILBENE	588590	0.	0.
1	8-METHYLQUINOLINE	611325	0.	0.
1	2-Furancarboxaldehyde,5-methyl-	620020	0.	0.
2	3-HYDROXY-4-METHOXYBENZALDEHYDE	621590	0.	0.
1	TEREPHTHALDEHYDE	623278	0.	0.
1	3-CHLOROPYRIDINE	626608	0.	0.
1	ADIPIC ACID-DIMETHYL ESTER	627930	0.	0.
2	1,1,3,3-TETRACHLORO-2-PROPANONE	632213	0.	0.
1	4-N-PROPYLPHENOL	645567	0.	0.
1	ISOPROPYLCYCLOHEXANE	696297	0.	0.

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Occurrences to Confirm	Compound name	CASRN	RTI Tentative Ident. %IND	Confirmations %CONF
1	S-ETHYL DIPROPYL THIOCARBAMATE	759944	0.	0.
1	Octanoicacid,8-hydroxy-	764896	0.	0.
1	Benzene,(1-methylheptyl)-	777220	0.	0.
1	3-INDOLEACETAMIDE	879378	0.	0.
1	PHENYLISOCYANIDE	931544	0.	0.
1	2-HYDROXYBENZOTHIAZOLE	934349	0.	0.
1	1,4,5,6,7,8,8-HEPTACHLORO-2,3-EPOXY	1024573	0.	0.
1	GLUTARIC ACID-DIMETHYL ESTER	1119400	0.	0.
3	TETRADECENE-1	1120361	0.	0.
1	2,4-DIMETHYL-6-ETHYLPYRIDINE	1124352	0.	0.
1	4-(2,5-XYLYL)BUTANOIC ACID	1453061	0.	0.
1	DIMETHYL ISOPHTHALATE	1459934	0.	0.
1	DIMETHYLAMINE PROPIONITRILE	1738256	0.	0.
2	1H-Indol-5-ol	1953544	0.	0.
1	1-NAPHTHYL-ISOCYANIDE	1984049	0.	0.
1	S-ETHYLDIISOBUTYLTHIOCARBAMATE	2008415	0.	0.
1	9-METHYLBENZO(A)ANTHRACENE	2381160	0.	0.
1	3-CHLOROCYCLOHEXENE	2441976	0.	0.
1	1-ALLYLNAPHTHALENE	2489863	0.	0.
2	9-METHYLFLUORENE	2523377	0.	0.
1	7-METHYLBENZO(A)ANTHRACENE	2541697	0.	0.
1	3-HYDROXY-1,2-BENZISOTHIAZOLE	2634335	0.	0.
1	3-METHYL-1,2-DIHYDRONAPHTHALENE	2717444	0.	0.
1	5-METHYLTETRALIN	2809645	0.	0.
2	AZELAIC ACID DI-N-BUTYL ESTER	2917739	0.	0.
1	Hexanoicacid,3,5,5-trimethyl-	3302101	0.	0.
1	6-METHYLINDOLE	3420028	0.	0.
2	2,3,5-TRIMETHYLPHENANTHRENE	3674735	0.	0.
2	5-METHYLCHRYSENE	3697243	0.	0.
1	METHYL HYDROGEN PHTHALATE	4376185	0.	0.
1	2-PHENYLTETRADECANE	4534592	0.	0.
1	1-METHYL-3-CYCLOHEXYLBENZENE	4575466	0.	0.
1	2,3-DIMETHYLFLUORENE	4612639	0.	0.
1	3-(4-HYDROXY-3-METHOXYPHENYL)-PROPA	4899745	0.	0.
1	HUMULENE	6753986	0.	0.
1	2-N-BUTYLQUINOLINE	7661394	0.	0.
1	2,5-DIISOPROPYL-P-XYLENE	10375969	0.	0.
1	2,7-DIMETHYL-1,2,3,4-TETRAHYDRONAPH	13065071	0.	0.
1	3-FUROIC ACID-METHYL ESTER	13129232	0.	0.
2	3-PHENYL-1,3-CYCLOHEXADIENE	15619348	0.	0.
1	2,6,2',6'-TETRACHLOROBIPHENYL	15968055	0.	0.
1	Cyclohexanol,2-bromo-,cis-	16536575	0.	0.
5	4,9-DIMETHYLNAPHTHO(2,3-B)THIOPHENE	16587341	0.	0.
1	2,5,4'-TRICHLOROBIPHENYL	16606023	0.	0.
1	1-Naphthylisocyanide,2-methyl-	20600571	0.	0.
2	SECONAL	22328945	0.	0.
2	2,3,4-TRIMETHYLCYCLOPENT-2-ENE-1-ON	28790865	0.	0.
1	2,4-DICHLOROBIPHENYL	33284503	0.	0.
1	2,5,2',5'-TETRACHLOROBIPHENYL	35693993	0.	0.
1	3,4,2'-TRICHLOROBIPHENYL	38444869	0.	0.
1	2,4,2',5'-TETRACHLOROBIPHENYL	41464408	0.	0.
1	AR-ETHYLBENZALDEHYDE	53951501	0.	0.
2	2,3,4 TRICHLORO BIPHENYL	55702460	0.	0.

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1	CHLORDENE(TENTATIVE FROM FIELD SAMP	56534033	0.	0.
1	1-BROMO-3-CHLOROBENZENE	108372	0.	100.
7	PENTACHLOROPHENOL	87865	14.	100.
12	STEARIC ACID	57114	16.	100.
5	PHTHALIC ACID	88993	20.	100.
5	3,5-DIMETHYL-BENZOIC ACID	499069	20.	100.
4	SYRINGIC ACID	530574	25.	0.
4	1-METHYL PYRENE	2381217	25.	0.
4	4,5-DIMETHYLPHENANTHRENE	3674699	25.	0.
4	4-METHYLDIBENZO(BD)FURAN	7320538	25.	0.
4	DIMETHYL SULPHOXIDE	67685	25.	100.
4	DIOCTYL ADIPATE	123795	25.	100.
4	1,8-CINEOLE	470826	25.	100.
4	2,3-DIHYDROBENZOFURAN	496162	25.	100.
4	TERPINOLENE	586629	25.	100.
4	2,4-DIMETHYLBENZOIC ACID	611018	25.	100.
4	N-OCTACOSANE	630024	25.	100.
7	1-HEXADECENE	629732	28.	50.
4	1-METHYL-7-ISOPROPYLNAPHTHALENE	490653	33.	0.
3	2,3-DIMETHYL-BENZOIC ACID	603792	33.	0.
3	6-METHYL-INDOLIZINE	1761111	33.	0.
4	1-METHYLBENZO(A)ANTHRACENE	2498773	33.	0.
3	2-METHYLCARBAZOLE	3652913	33.	0.
3	SULFUR	7704349	33.	0.
3	3-HYDROXYBENZOIC ACID-METHYL ESTER	19438109	33.	0.
3	2-ETHYLANTHRACENE	52251715	33.	0.
6	3,4-DICHLOROBENZOIC ACID	51445	33.	100.
3	CHOLESTEROL	57885	33.	100.
3	PHTHALIDE	87412	33.	100.
6	BENZALDEHYDE	100527	33.	100.
3	P-CHLOROPHENOL	106489	33.	100.
3	P-HYDROXY-BENZALDEHYDE	123080	33.	100.
6	2-HYDROXY-2-METHYL-4-PENTANONE	123422	33.	100.
3	MESITYL OXIDE	141797	33.	100.
3	9H-Fluoren-9-one	486259	33.	100.
3	M-CHLOROBENZOIC ACID	535808	33.	100.
3	2,5-DIMETHYL-BENZOIC ACID	610720	33.	100.
3	TRIACONTANE	638686	33.	100.
3	2-ACETYLPYRROLE	1072839	33.	100.
3	1-TRIDECENE	2437561	33.	100.
8	2,3-DIMETHYLPHENANTHRENE	3674655	37.	0.
8	O-ETHYLPHENOL	90006	37.	100.
21	PALMITIC ACID	57103	38.	87.
13	PHENYLPROPIONIC ACID	501520	38.	100.
5	O-NITROPHENOL	88755	40.	100.
5	METHYL BENZOATE	93583	40.	100.
5	1-OCTADECANOL	112925	40.	100.
18	MYRISTIC ACID	544638	41.	100.
7	4-HYDROXY-3-METHOXY-PHENYLACETIC AC	306081	42.	66.
7	2-METHYLBIPHENYL	643583	42.	66.
9	NICOTINE	54115	42.	100.
26	BENZOIC ACID	65850	42.	100.
7	LIMONENE	138863	42.	100.

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9	ANILINE	62533	44.	100.
6	3-CHLORO-2-HYDROXYTOLUENE	87649	50.	0.
2	2,4-DIHYDROXYACETOPHENONE	89849	50.	0.
2	1-HYDROXY-3,4-DIMETHYLBENZENE(3,4-D	95658	50.	0.
2	GAMMA TERPINENE	99854	50.	0.
2	DICYCLOHEXYLAMINE	101837	50.	0.
2	4-METHYLPYRIDINE	108894	50.	0.
2	NAPHTHOL(2,1-B)THIANAPHTHENE	205436	50.	0.
2	BENZO(C)CINNOLINE	230171	50.	0.
2	CAPROLACTONE	502443	50.	0.
2	2-BENZYLNAPHTHALENE	613592	50.	0.
2	2,2-DIFURYLMETHANE	1197406	50.	0.
4	3-METHYL-INDOLIZINE	1761100	50.	0.
2	4,5-DICHLOROGUAIACOL	2460493	50.	0.
6	2,5-DIMETHYLPHENANTHRENE	3674666	50.	0.
2	1,1,3-TRIMETHYL-3-PHENYLINDAN	3910358	50.	0.
2	3-ETHYL-5-METHYLPYRIDINE	3999788	50.	0.
2	4-PHENYLCYCLOHEXENE	4994165	50.	0.
2	AROCHLOR-1254-1 (TETRACHLOROBIPHENY	11097691	50.	0.
2	5-METHYL-2,3-BENZOTHIOPHENE	14315141	50.	0.
2	BIS-(2-CHLOROISOPROPYL) ETHER	39638329	50.	0.
2	P-(2,2,3,3-TETRAMETHYLBUTYL)PHENOL	54932784	50.	0.
2	ACETIC ACID	64197	50.	100.
2	CHLOROFORM	67663	50.	100.
2	HEXACHLOROETHANE	67721	50.	100.
4	SALICYLIC ACID	69727	50.	100.
2	TRIETHYL PHOSPHATE	78400	50.	100.
8	DIETHYL PHTHALATE	84662	50.	100.
2	SALICYLALDEHYDE	90028	50.	100.
4	1-CHLORONAPTHALENE	90131	50.	100.
2	2-AMINONAPHTHALENE	91598	50.	100.
2	BENZANILIDE	93981	50.	100.
2	INDENE	95136	50.	100.
4	1-HYDROXY-2,5-DIMETHYLBENZENE	95874	50.	100.
2	ALPHA-METHYLSTYRENE	98836	50.	100.
2	2,6-DICHLORO-4-NITROANILINE	99309	50.	100.
2	1,3-DIISOPROPYLBENZENE	99627	50.	100.
3	P-TOLUIC ACID,METHYL ESTER	99752	50.	100.
4	BENZONITRILE (CYANOBENZENE)	100470	50.	100.
2	AZOBENZENE	103333	50.	100.
2	DIBENZYLAMINE	103491	50.	100.
2	2-PHENYLACETAMIDE	103811	50.	100.
2	BIS(2-CHLOROETHYL)ETHER	111444	50.	100.
4	DODECANOL	112538	50.	100.
2	OLEIC ACID-METHYL ESTER	112629	50.	100.
8	O-TOLUIC ACID	118901	50.	100.
11	DIBENZOTHIOPHENE	132650	50.	100.
6	SYRINGALDEHYDE (4-HYDROXY-3,5-DIMET	134963	50.	100.
4	2-NAPHTHOL	135193	50.	100.
2	3-PHENYL-1-PROPENE (ALLYLBENZENE)	300572	50.	100.
4	Naphthalene,1-phenyl-	605027	50.	100.
2	META-ISOPROPYLPHENOL	618451	50.	100.
6	3,4-DIMETHYL-BENZOIC ACID	619045	50.	100.

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2	N-HENEICOSANE	629947	50.	100.
2	TRIDECANOIC ACID	638539	50.	100.
4	PENTAMETHYLBENZENE	700129	50.	100.
2	GAMMA-DECALACTONE	706149	50.	100.
2	2,2,4,4-TETRAMETHYL-3-PENTANONE	815247	50.	100.
2	METHYL HEPTYL KETONE	821556	50.	100.
2	2,6-DIMETHYLQUINOLINE	877430	50.	100.
2	4-METHYLFLUORENE	1556996	50.	100.
7	2,7-DIMETHYLPHENANTHRENE	1576698	50.	100.
2	ACETOSYRINGONE	2478388	50.	100.
4	2-METHYLPYRENE	3442782	50.	100.
2	DIPROPYLENEGLYCOL METHYL ETHER	12002254	50.	100.
2	PARA-ALPHA-CUMYLPHENOL	22239549	50.	100.
11	3-METHYLPHENANTHRENE	832713	54.	0.
11	FLUORENE	86737	54.	83.
11	1-METHYLFLUORENE	1730376	54.	83.
10	2-(2-ETHOXYETHOXY) ETHANOL	111900	55.	100.
8	3-METHYLDIBENZOTHIOPHENE	16587523	57.	0.
7	3,6-DIMETHYLPHENANTHRENE	1576676	57.	100.
12	VANILLIN (4-HYDROXY-3-METHOXY BENZA	121335	58.	100.
13	PYRENE (BENZOPHENANTHRENE)	129000	58.	100.
5	3-METHYLPYRIDINE	108996	60.	0.
5	P-TOLUENESULPHONAMIDE	70553	60.	66.
10	2-METHYL ANTHRACENE	613127	60.	66.
16	PHENANTHRENE	85018	60.	100.
6	CARBAZOLE	86748	60.	100.
5	DIPHENYLMETHANE	101815	60.	100.
5	CHRYSENE	218019	60.	100.
5	1-HYDROXY-2,3-DIMETHYLBENZENE	526750	60.	100.
5	M-DICHLOROBENZENE	541731	60.	100.
11	N-TRICOSANE	638675	60.	100.
13	DIOCTYL PHTHALATE	117840	61.	50.
13	ACETOPHENONE	98862	61.	87.
18	PHENYLACETIC ACID	103822	61.	90.
13	BIPHENYL	92524	61.	100.
13	DECANOIC ACID	334485	61.	100.
8	2-METHYLPHENANTHRENE	2531842	62.	60.
8	ACENAPHTHENE	83329	62.	80.
9	M-DIETHYLBENZENE	141935	62.	100.
8	4-HYDROXY-3-METHOXYACETOPHENONE	498022	62.	100.
11	M-TOLUIC ACID	99047	63.	85.
24	DI-(2-ETHYLHEXYL)PHTHALATE	117817	65.	86.
3	O-TERPHENYL	84151	66.	0.
3	O-TERT BUTYL PHENOL	88186	66.	0.
12	1,7-DIMETHYLNAPHTHALENE	575371	66.	0.
3	9,10-DIMETHYLPHENANTHRENE	604831	66.	0.
3	METHYLPHENYLACETYLENE	673325	66.	0.
3	1,3-DIMETHYL-2-ETHYLBENZENE	2870044	66.	0.
3	1-ISOPROPYL-2,5-DIMETHYLBENZENE	4132723	66.	0.
22	1,8-DIMETHYLNAPHTHALENE	569415	66.	7.
3	ALPHA-PINENE	80568	66.	50.
3	METHYL LINOLENATE	112630	66.	50.
3	3,4-DIMETHOXY PHENOL	2033898	66.	50.

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3	2-METHYLDECANE	6975980	66.	50.
6	ORTHO-ISOPROPYLPHENOL (ORTHO-CUMENO	88697	66.	75.
6	Benzoicacid,4-(1,1-dimethylethyl)-	98737	66.	75.
6	O-METHYLSTYRENE	611154	66.	75.
16	ISOPROPYLBENZENE	98828	66.	81.
10	FLUORANTHENE	206440	66.	83.
9	9-METHYLPHENANTHRENE	883205	66.	83.
9	BENZENE	71432	66.	100.
6	CAMPHOR	76222	66.	100.
3	PROPANOIC ACID(PROPIONIC ACID)	79094	66.	100.
6	BUTYL BENZYL PHTHALATE	85687	66.	100.
3	1-PHENYLETHANOL	98851	66.	100.
3	P-NONYLPHENOL	104405	66.	100.
3	TRI-PHENYL PHOSPHATE	115866	66.	100.
3	3-PHENYLPROPANOL	122974	66.	100.
3	1,4-DIOXANE	123911	66.	100.
3	DIMETHYL PHTHALATE	131113	66.	100.
3	1,2-DIETHYLBENZENE	135013	66.	100.
3	2,4,6-TRIMETHYLPHENOL	527606	66.	100.
6	1-HYDROXY-2,6-DIMETHYLBENZENE(2,6-D	576261	66.	100.
6	2,3-DIMETHYLNAPHTHALENE	581408	66.	100.
3	2-PHENYLNAPHTHALENE	612942	66.	100.
3	2(METHYLTHIO)BENZOTHIAZOLE	615225	66.	100.
3	3-METHYLCYCLOPENT-2-ENE-1-ONE	2758181	66.	100.
3	4-METHYLDECANE	2847725	66.	100.
17	HEXANOIC ACID(CAPROIC ACID)	142621	68.	100.
17	O-CRESOL	95487	70.	83.
11	CAFFEINE	58082	70.	100.
10	NONANOIC ACID	112050	70.	100.
17	2,3,6-TRIMETHYLNAPHTHALENE	829265	70.	100.
11	1-ISOPROPYL-3,5-DIMETHYLBENZENE	4706905	70.	100.
7	2-METHYL-2,4-PENTANEDIOL	107415	71.	100.
8	2-PHENOXYETHANOL	122996	71.	100.
7	FENCHYL ALCOHOL	1632731	71.	100.
11	(2,6-DI-TERT-BUTYL-4-METHYL PHENOL)	128370	72.	100.
11	1-METHYL-2-N-PROPYLBENZENE	1074175	72.	100.
16	2-N-BUTOXYETHANOL	111762	73.	100.
15	OCTANOIC ACID	124072	73.	100.
4	4-METHYL-(2,3-DIHYDROINDENE)(4-METH	824226	75.	0.
4	3,4,5-TRIMETHYLPHENOL	527548	75.	33.
5	ISOPHORONE	78591	75.	66.
4	P-ISOPROPYLPHENOL	99898	75.	66.
4	5-METHYL-(2,3-DIHYDROINDENE)(5-METH	874351	75.	66.
4	1,2-DIMETHYL-4-ETHYLBENZENE	934805	75.	66.
17	STYRENE	100425	75.	75.
8	FURFURYL ALCOHOL	98000	75.	80.
8	HEPTANOIC ACID	111148	75.	83.
16	LAURIC ACID	143077	75.	91.
4	1,2-BENZANTHRACENE	56553	75.	100.
4	INDAN-1-ONE	83330	75.	100.
5	1-TETRADECANOL	112721	75.	100.
5	1,2,3,5-TETRAMETHYLBENZENE	527537	75.	100.
13	1,4-DIMETHYLNAPHTHALENE	571584	75.	100.

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4	2,6-DIMETHYLNAPHTHALENE	581420	75.	100.
8	1-METHYLPHENANTHRENE	832699	75.	100.
14	O-CYMENE	527844	76.	50.
13	1,3,5-TRIMETHYLBENZENE	108678	76.	90.
9	SEC-BUTYLBENZENE	135988	77.	85.
14	2,3,5-TRIMETHYLNAPHTHALENE	2245387	78.	81.
33	2-(2-BUTOXYETHOXY) ETHANOL	112345	78.	96.
19	ALPHA-TERPINEOL	98555	78.	100.
14	NONADECANE	629925	78.	100.
11	1-METHYL-(2,3-DIHYDROINDENE) (1-MET	767588	80.	0.
10	2-METHYLINDAN	824635	80.	0.
5	METHYL DEHYDROABIETATE	1235741	80.	0.
5	1,2-DIMETHYLINDAN	17057828	80.	0.
5	META-ETHYLPHENOL	620177	80.	75.
21	2-ETHYL-1-HEXANOL	104767	80.	87.
10	1,2,3,4-TETRAMETHYLBENZENE (PREHNIT	488233	80.	87.
5	2,4,6-TRICHLOROPHENOL	88062	80.	100.
5	STEARIC ACID METHYL ESTER	112618	80.	100.
5	2,4-DICHLOROPHENOL	120832	80.	100.
5	INDANE	496117	80.	100.
20	N-OCTADECANE	593453	80.	100.
18	META-CRESOL (3-METHYLPHENOL)	108394	81.	92.
11	PHENYL ETHER	101848	81.	100.
16	N-EICOSANE	112958	81.	100.
17	HEPTADECANE	629787	82.	100.
6	BIPHENYLENE	259790	83.	60.
6	Benzene,1,2-dichloro-	95501	83.	100.
6	4-METHYL-2-PENTANONE	108101	83.	100.
12	PENTANOIC ACID (VALERIC ACID)	109524	83.	100.
6	METHYL N-HEXADECANOATE	112390	83.	100.
18	2,7-DIMETHYLNAPHTHALENE	582161	83.	100.
6	1-ETHYLNAPHTHALENE	1127760	83.	100.
6	4,7-DIMETHYLINDAN	6682719	83.	100.
14	PARA-CRESOL (4-METHYLPHENOL)	106445	84.	90.
14	1,3,6-TRIMETHYLNAPHTHALENE	3031081	85.	0.
7	2,4,5-TRICHLOROPHENOL	95954	85.	83.
14	DIBUTYL PHTHALATE	84742	85.	100.
20	1,4-DIMETHYLBENZENE(P-XYLENE)	106423	85.	100.
7	INDOLE	120729	85.	100.
20	PENTADECANE	629629	85.	100.
16	1,5-DIMETHYLNAPHTHALENE	571619	86.	100.
8	N-PROPYLBENZENE	103651	87.	85.
17	1,2,4-TRIMETHYLBENZENE	95636	87.	100.
10	N-BUTANOIC ACID(BUTYRIC ACID)	107926	87.	100.
8	PARA-ETHYLPHENOL	123079	87.	100.
17	N-TRIDECANE	629505	87.	100.
9	2,4-XYLENOL	105679	88.	75.
9	O-HYDROXYDIPHENYL	90437	88.	87.
18	TOLUENE	108883	88.	93.
20	1-METHYL-4-ETHYLBENZENE	622968	88.	93.
9	BENZOTHIAZOLE	95169	88.	100.
17	ETHYLBENZENE	100414	88.	100.
20	NOR-DODECANE	112403	89.	88.

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Occurrences to Confirm	Compound name	CASRN	RTI Tentative Ident. %IND	Confirmations %CONF
19	1-METHYL-2-ETHYLBENZENE	611143	89.	94.
20	TETRACHLOROETHYLENE	127184	89.	100.
22	1-METHYL NAPHTHALENE	90120	90.	100.
21	2-METHYLNAPHTHALENE	91576	90.	100.
21	PHENOL	108952	90.	100.
13	BENZYL ALCOHOL	100516	91.	90.
12	1,6-DIMETHYLNAPHTHALENE	575439	91.	100.
14	ANTHRACENE	120127	92.	92.
25	NAPHTHALENE	91203	92.	100.
14	5-ETHYL-M-XYLENE	934747	92.	100.
13	2-ETHYLNAPHTHALENE	939275	92.	100.
17	P-CYMENE	99876	93.	69.
16	1,3-DIMETHYLNAPHTHALENE	575417	93.	100.
16	1-METHYL-3-ETHYLBENZENE	620144	93.	100.
18	1,2,3-TRIMETHYLBENZENE	526738	94.	93.
19	N-TETRADECANE	629594	94.	100.
21	N-HEXADECANE	544763	95.	100.
1	1,1,3,3,5-PENTAMETHYL-(2,3-DIHYDROI	81038	100.	0.
1	BUTYL (BUTOXYCARBONYL)METHYL PHTHAL	85701	100.	0.
1	9H-Thioxanthen-9-one,2-chloro-	86395	100.	0.
1	4-AMINOBIPHENYL	92671	100.	0.
2	4-NITROBIPHENYL	92933	100.	0.
2	TERT-BUTYLBENZENE	98066	100.	0.
1	2-CHLORO-4-TERT-BUTYLPHENOL	98282	100.	0.
1	2-PHENYLPROPENE	98839	100.	0.
1	DI-P-TOLYL DISULFIDE	103195	100.	0.
1	ALPHA-CHLORO-P-XYLENE	104825	100.	0.
1	BIS-(2-ETHYLHEXYL)AMINE	106207	100.	0.
1	DI-N-BUTYLAMINE	111922	100.	0.
1	Phenol,2,6-bis(1,1-dimethylethyl)-	128392	100.	0.
1	BETA-TERPINEOL	138874	100.	0.
2	2-MERCAPTOBENZOTHIAZOLE	149304	100.	0.
1	2,13-BENZFLUORANTHENE	203123	100.	0.
2	10,11-BENZFLUORANTHENE	205823	100.	0.
1	NAPHTHO(1,2-B)THIANAPHTHENE	239350	100.	0.
1	CYCLOFENCHENE	488971	100.	0.
1	4-TERT-BUTYL-2-PHENYLPHENOL	577924	100.	0.
2	ALPHA-HYDROXY-O-TOLUIC ACID	612204	100.	0.
1	3,3PRIME-DIMETHYLBIPHENYL	612759	100.	0.
1	4,4'-DIMETHYLBIPHENYL	613332	100.	0.
1	4-CHLORO-O-XYLENE	615601	100.	0.
1	P-CHLOROBENZAMIDE	619567	100.	0.
1	BICYCLO(4.2.0)OCTA-1,3,5-TRIENE	694871	100.	0.
2	2,3,5-TRIMETHYLPYRIDINE	695987	100.	0.
1	1,4-DICHLORO-2-BUTENE	764410	100.	0.
1	3-METHYLINDENE	767602	100.	0.
1	ISOLONGIFOLENE	1135666	100.	0.
1	AR,ALPHA-DIMETHYLSTYRENE	1195320	100.	0.
1	O-ALLYLTOLUENE	1587048	100.	0.
1	SANDARACOPIMARADIENE	1686562	100.	0.
1	ISOPIMARADIENE	1686664	100.	0.
1	1-HYDROXY-3-METHYL-6-ETHYLBENZENE	1687612	100.	0.
3	1,4-DIMETHYL-2-ETHYLBENZENE	1758889	100.	0.

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1	TRIMETHYLETHYLLEAD	1762261	100.	0.
1	DIMETHYLDIETHYLLEAD	1762272	100.	0.
1	4,4-DICHLOROBIPHENYL	2050682	100.	0.
1	5-METHYLBENZ(A)ANTHRACENE	2319962	100.	0.
1	1,2-DIPHENYLBENZIMIDAZOLE	2622675	100.	0.
2	2,4-DIISOPROPYLPHENOL	2934056	100.	0.
1	4-METHYLPYRENE	3353126	100.	0.
1	SABINENE	3387415	100.	0.
1	2,3,4-TRITHIAPENTANE	3658808	100.	0.
1	1,2-HEPTANEDIOL	3710314	100.	0.
1	2,6-DI-TERT-BUTYLNAPHTHALENE	3905644	100.	0.
1	2-BUTYL-1-OCTANOL	3913028	100.	0.
1	2-ISOPROPYLTHIOPHENE	4095221	100.	0.
1	2-METHYLBENZOFURAN	4265252	100.	0.
1	DIFURFURYL ETHER	4437223	100.	0.
2	1-ISOPROPYL-2,4-DIMETHYLBENZENE	4706892	100.	0.
1	1,1-DIMETHYLINDAN	4912929	100.	0.
1	METHYL 14-METHYL PENTADECANOATE	5129602	100.	0.
1	3,4-DIMETHYLBENZALDEHYDE	5973717	100.	0.
1	4-METHYLDIBENZOTHIOPHENE	7372885	100.	0.
1	1,2,4-TRIMETHYL-5-ISOPROPYLBENZENE	10222954	100.	0.
1	2,5-DIMETHYL-3-ETHYL PYRAZINE	13360651	100.	0.
1	1,4-DICHLOROBUTENE-1	13676589	100.	0.
1	2-ETHYL-6-METHYLPYRAZINE	13925036	100.	0.
2	1-CHLORO-3,5-DIBROMOBENZENE	14862523	100.	0.
1	2,4,5-TRICHLOROBIPHENYL	15862074	100.	0.
1	2,7-DIMETHYLBENZO(B)THIOPHENE	16587409	100.	0.
1	3,6-DIMETHYL-1-THIAINDENE	16587501	100.	0.
1	2,4,5-TRIMETHYLETHYLBENZENE	17851273	100.	0.
1	EPIJUVABIONE	17904277	100.	0.
1	DEHYDROABIETANE	19407284	100.	0.
1	1,3-DICHLORO-5-BROMOBENZENE	19752557	100.	0.
1	5-HYDROXY-2-METHYLPYRIMID-4-ONE	24614140	100.	0.
1	PIPERIDONE	27154434	100.	0.
1	2-METHYLTEREPHTHALDEHYDE	27587173	100.	0.
1	2-METHYL-5-PROPYLTHIOPHENE	33933732	100.	0.
1	PENTACHLOROPROPENE	34774691	100.	0.
1	2,5,3' TRICHLORO BIPHENYL	38444814	100.	0.
1	1,1,5-TRIMETHYLINDANE	40650417	100.	0.
1	DIBUTYL ORTHOFORMATE	54518046	100.	0.
2	3,4-BENZPYRENE	50328	100.	0.
2	1-NAPHTHOL	90153	100.	50.
2	M-AMINOACETOPHENONE	99036	100.	50.
2	ALPHA TERPINENE	99865	100.	50.
2	P-DIISOPROPYLBENZENE	100185	100.	50.
2	P-ANISIDINE	104949	100.	50.
2	1,3,5-TRICHLOROBENZENE	108703	100.	50.
2	1-CHLORO-3-NITROBENZENE	121733	100.	50.
2	M-TERT-BUTYLPHENOL	585342	100.	50.
2	Phenol,2,3,6-trichloro-	933755	100.	50.
10	2-ISOPROPYLNAPHTHALENE	2027170	100.	50.
3	2,3-BENZOTHIOPENE (THIANAPHTHENE)	95158	100.	66.
3	2-METHYLINDOLE	95205	100.	66.

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3	3,4-DICHLOROANILINE	95761	100.	66.
3	2-METHYLPYRIDINE	109068	100.	66.
3	HEPTAN-2-ONE	110430	100.	66.
3	2,3 BENZOFLUORENE	243174	100.	66.
3	2,4,5-TRIMETHYLPHENOL	496786	100.	66.
3	1,2-DIMETHYLNAPHTHALENE	573988	100.	66.
3	1-METHYL-3-N-PROPYLBENZENE	1074437	100.	66.
7	1,2,4,5-TETRAMETHYLBENZENE	95932	100.	71.
4	O-TOLUIDINE	95534	100.	75.
6	QUINOLINE (1-BENZAZINE)	91225	100.	80.
5	3-ETHYL-O-XYLENE	933982	100.	80.
6	2,3,4,6-TETRACHLOROPHENOL	58902	100.	83.
8	1,3-DIMETHYL-4-ETHYLBENZENE	874419	100.	85.
9	BORNEOL	507700	100.	88.
10	1-METHYL-3-ISOPROPYLBENZENE	535773	100.	88.
18	1,3-DIMETHYLBENZENE(M-XYLENE)	108383	100.	94.
2	4-CHLORO-M-CRESOL	59507	100.	100.
1	4-AMINO-AZOBENZENE	60093	100.	100.
5	2-PHENYL ETHANOL	60128	100.	100.
1	DIELDRIN	60571	100.	100.
3	DIMETHYL SULFONE	67710	100.	100.
1	N,N-DIMETHYLFORMAMIDE	68122	100.	100.
1	1-BUTANOL	71363	100.	100.
1	1,1,1-TRICHLOROETHANE	71556	100.	100.
1	TETRAMETHYLLEAD	75741	100.	100.
1	1,1,2-TRICHLOROETHANE	79005	100.	100.
2	TRICHLOROETHYLENE	79016	100.	100.
4	ISOBUTYRIC ACID	79312	100.	100.
1	METHACRYLIC ACID	79414	100.	100.
1	CAMPHENE	79925	100.	100.
1	BENZANTHRONE	82053	100.	100.
2	3-METHYLINDOLE	83341	100.	100.
2	9,10-ANTHRAQUINONE	84651	100.	100.
1	DIISOBUTYL PHTHALATE	84695	100.	100.
1	DINONYL PHTHALATE	84764	100.	100.
1	3,4,5-TRIMETHOXYBENZALDEHYDE	86817	100.	100.
4	1,2,3-TRICHLOROBENZENE	87616	100.	100.
1	2,6-DICHLOROPHENOL	87650	100.	100.
1	ORTHO-NITROTOLUENE	88722	100.	100.
1	4-CHLORO-2-NITROANILINE	89634	100.	100.
1	PIPERITONE	89816	100.	100.
1	O-METHYLBENZYL ALCOHOL	89952	100.	100.
5	ORTHO-METHOXYPHENOL	90051	100.	100.
1	1-Naphthalenamine,N-phenyl-	90302	100.	100.
1	1,2-DIMETHOXYBENZENE (VERATROLE)	91167	100.	100.
2	PHENOTHIAZINE	92842	100.	100.
1	PROPIOPHENONE	93550	100.	100.
4	SAFROLE	94597	100.	100.
14	1,2-DIMETHYLBENZENE(O-XYLENE)	95476	100.	100.
4	1-METHYL-2-CHLOROBENZENE (O-CHLOROT	95498	100.	100.
1	2-CHLOROANILINE	95512	100.	100.
1	O-BROMOPHENOL	95567	100.	100.
2	O-CHLOROPHENOL	95578	100.	100.

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1	2,4-DICHLOROTOLUENE	95738	100.	100.
1	3,4-DICHLOROTOLUENE	95750	100.	100.
1	1,2,4,5-TETRACHLOROBENZENE	95943	100.	100.
1	EPOXYETHYL BENZENE (STYRENE OXIDE)	96093	100.	100.
2	2,4-DI-TERT-BUTYLPHENOL	96764	100.	100.
1	EUGENOL	97530	100.	100.
1	2-METHOXY-4-(PROP-2-ENYL)-PHENOL	97541	100.	100.
5	FURFURAL	98011	100.	100.
6	P-TERT BUTYLPHENOL	98544	100.	100.
5	NITROBENZENE	98953	100.	100.
1	1,3-DINITROBENZENE	99650	100.	100.
1	PARA-NITROTOLUENE	99990	100.	100.
1	P-NITROANILINE	100016	100.	100.
2	2-VINYLPYRIDINE	100696	100.	100.
1	2-ETHYLPYRIDINE	100710	100.	100.
1	2-METHYL-5-ETHYLPYRIDINE	104905	100.	100.
1	P-ANISYLALCOHOL	105135	100.	100.
3	ETHYL LAURATE	106332	100.	100.
1	P-BROMOPHENOL	106412	100.	100.
5	P-DICHLOROBENZENE	106467	100.	100.
1	1,2-DIBROMOETHANE	106934	100.	100.
1	CHLOROETHANENITRILE	107142	100.	100.
2	M-CHLOROANILINE	108429	100.	100.
1	M-CHLOROPHENOL	108430	100.	100.
1	2,6-DIMETHYLPYRAZINE	108509	100.	100.
6	3,5-XYLENOL	108689	100.	100.
1	2,4,6-TRIMETHYL PYRIDINE	108758	100.	100.
1	CHLOROBENZENE	108907	100.	100.
1	CYCLOHEXANONE	108941	100.	100.
1	BENZENETHIOL (THIOPHENOL)	108985	100.	100.
1	METHYL CAPRATE	110429	100.	100.
1	BUTYNE-1,4-DIOL	110656	100.	100.
1	2-ETHOXYETHANOL	110805	100.	100.
2	CYCLOHEXENE	110838	100.	100.
2	PYRIDINE	110861	100.	100.
1	OCTANOIC ACID-METHYL ESTER	111115	100.	100.
1	2-(2-METHOXYETHOXY)ETHANOL	111773	100.	100.
1	METHYL LAURATE	111820	100.	100.
2	2-UNDECANONE	112129	100.	100.
2	2-HEXYLOXYETHANOL	112254	100.	100.
1	1-UNDECANOL	112425	100.	100.
1	2-METHYL-3-BUTYN-2-OL	115195	100.	100.
1	O-HYDROXYACETOPHENONE	118934	100.	100.
2	2-NITRO-P-CRESOL	119335	100.	100.
3	BENZOPHENONE	119619	100.	100.
1	ISOQUINOLINE	119653	100.	100.
2	DIMETHYLTEREPHTHALATE	120616	100.	100.
1	2-METHYLBENZOTHIAZOLE	120752	100.	100.
5	1,2,4-TRICHLOROBENZENE	120821	100.	100.
1	2,4-DINITROTOLUENE	121142	100.	100.
4	DIPHENYLAMINE	122394	100.	100.
1	3-METHYL-1-BUTANOL	123513	100.	100.
1	PARALDEHYDE	123637	100.	100.

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3	ETHYL MYRISTATE	124061	100.	100.
2	METHYL TETRADECANOATE	124107	100.	100.
10	N-DECANE	124185	100.	100.
5	TRI-BUTYL PHOSPHATE	126738	100.	100.
4	DIBENZOFURAN	132649	100.	100.
1	DIPHENYL SULFIDE	139662	100.	100.
1	BENZYL ACETATE	140114	100.	100.
1	P-ALLYLANISOLE	140670	100.	100.
1	NEROLIDOL	142507	100.	100.
3	TRIETHYLENE GLYCOL N-BUTYL ETHER	143226	100.	100.
1	TETRAETHYLENE GLYCOL DIMETHYL ETHER	143248	100.	100.
2	2,2,4-TRIMETHYLDIHYDROQUINOLINE	147477	100.	100.
1	2,4,6-TRIBROMOANILINE	147820	100.	100.
1	P-METHOXYPHENOL	150765	100.	100.
1	P-DIMETHOXYBENZENE	150787	100.	100.
1	PERYLENE	198550	100.	100.
2	4,5-METHYLENEPHENANTHRENE	203645	100.	100.
2	BENZO(K)FLUORANTHENE	207089	100.	100.
2	ACENAPHTHALENE	208968	100.	100.
1	TRIPHENYLENE	217594	100.	100.
1	BENZOFURAN	271896	100.	100.
1	1,3,5-TRITHIANE	291214	100.	100.
1	O-FLUOROPHENOL	367124	100.	100.
1	LONGIFOLENE	475207	100.	100.
1	THIAXANTHONE	492228	100.	100.
3	P-CYMEN-ALPHA-OL	499752	100.	100.
1	2,6-DIMETHYL-2,5-HEPTADIEN-4-ONE	504201	100.	100.
3	1-TETRALONE	529340	100.	100.
1	P-IODOPHENOL	540385	100.	100.
1	2,4-DICHLOROANILINE	554007	100.	100.
2	TERPINENE-4-OL	562743	100.	100.
1	4-METHYLCYCLOHEXANONE	589924	100.	100.
2	2-TRIDECANONE	593088	100.	100.
3	N-HEPTACOSANE	593497	100.	100.
1	2,6-DINITROTOLUENE	606202	100.	100.
1	2,3-DICHLOROANILINE	608275	100.	100.
1	1,1-DIPHENYLETHANE	612000	100.	100.
1	METHYLPHENYLNITROSOAMINE	614006	100.	100.
1	5-METHYLINDOLE	614960	100.	100.
1	2,3-DICHLORO-1-PROPANOL	616239	100.	100.
2	2-PHENYL-2-PROPANOL	617947	100.	100.
1	CINNAMIC ACID	621829	100.	100.
2	2,3-DITHIABUTANE	624920	100.	100.
3	PALMITIC ACID-ETHYL ESTER	628977	100.	100.
2	N-DOCOSANE	629970	100.	100.
6	N-PENTACOSANE	629992	100.	100.
3	N-HEXACOSANE	630013	100.	100.
1	1,1,1,2-TETRACHLOROETHANE	630206	100.	100.
1	1,2,3-TRIMETHOXYBENZENE	634366	100.	100.
1	PROPENYLBENZENE	637503	100.	100.
1	1-BROMO-2-CHLOROBENZENE	694804	100.	100.
2	2,3,5-TRIMETHYLPHENOL	697825	100.	100.
1	2,6-DI-TERT-BUTYL-P-BENZOQUINONE	719222	100.	100.

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2	METHYL-1-INDENE	767599	100.	100.
1	TRIPHENYLPHOSPHINE OXIDE	791286	100.	100.
2	TRANS,1,2-DICHLOROCYCLOHEXANE	822866	100.	100.
1	N-METHYL-2-PYRROLIDONE	872504	100.	100.
1	DIPHENYL DISULFIDE	882337	100.	100.
7	N-UNDECANE	1120214	100.	100.
2	FENCHONE	1195795	100.	100.
1	MENTHOL	1490046	100.	100.
1	4,6-DICHLORO-O-CRESOL	1570656	100.	100.
1	2,4,6-TRIMETHYLACETOPHENONE	1667012	100.	100.
1	ETHYL-CYCLOHEXANE	1678917	100.	100.
3	4,6-DIMETHYLINDAN	1685821	100.	100.
1	ATRAZINE	1912249	100.	100.
2	2,6,10,14-TETRAMETHYL PENTADECANE	1921706	100.	100.
1	2,6-DIISOPROPYL PHENOL	2078548	100.	100.
1	4-ETHYLRESORCINOL	2896608	100.	100.
1	2,3-DICHLORONITROBENZENE	3209221	100.	100.
1	N-BUTYLBENZENESULPHONAMIDE	3622842	100.	100.
1	2-BUTENAL (CROTONALDEHYDE)	4170303	100.	100.
1	1,2-BIS(METHYLMERCAPTO)ETHANE	6628188	100.	100.
1	SQUALENE	7683649	100.	100.
3	DELTA-3-CARENE	13466789	100.	100.
1	TRIMETHYL PYRAZINE	14667551	100.	100.
3	BETA PINENE	18172673	100.	100.
1	TRIPROPYLENE GLYCOL METHYL ETHER	20324338	100.	100.
1	BUTYLATED HYDROXY ANISOLE	25013165	100.	100.
1	TRANS-4-CHLOROCYCLOHEXANOL	29538770	100.	100.
2	1,4-DIBROMOCYCLOHEXANE	35076927	100.	100.
1	AR-BROMOPHENYL PHENYL ETHER	36563470	100.	100.
3	1-HEXADECANOL	36653824	100.	100.